



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:09 AM UTC

PDB ID : 8JFG / pdb_00008jfg
Title : Crystal structure of 3-oxoacyl-ACP reductase FabG in complex with NADP+ and 3-keto-octanoyl-ACP from Helicobacter pylori
Authors : Zhou, J.S.; Zhang, L.
Deposited on : 2023-05-18
Resolution : 2.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

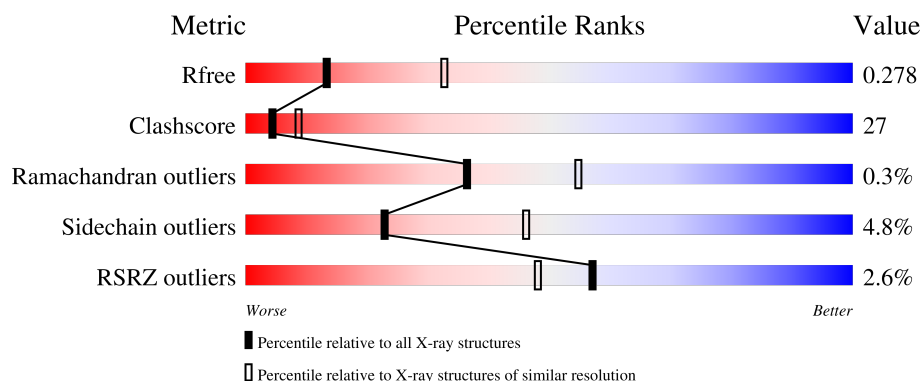
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	248	2% 65% 31% .
1	B	248	% 62% 29% 5%
1	C	248	2% 58% 34% .
1	D	248	3% 48% 43% 5%
1	E	248	3% 56% 38% .

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Mol	Chain	Length	Quality of chain
1	F	248	4% 54% 40% 2%
2	G	78	1% 29% 46% 15% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11747 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1875	1179	323	363	10			
1	B	236	Total	C	N	O	S	0	0	0
			1780	1122	307	342	9			
1	C	239	Total	C	N	O	S	0	0	0
			1803	1135	310	348	10			
1	D	236	Total	C	N	O	S	0	0	0
			1780	1122	307	342	9			
1	E	241	Total	C	N	O	S	0	0	0
			1821	1147	313	352	9			
1	F	239	Total	C	N	O	S	0	0	0
			1803	1135	310	348	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP G2M827
B	0	SER	-	expression tag	UNP G2M827
C	0	SER	-	expression tag	UNP G2M827
D	0	SER	-	expression tag	UNP G2M827
E	0	SER	-	expression tag	UNP G2M827
F	0	SER	-	expression tag	UNP G2M827

- Molecule 2 is a protein called Acyl carrier protein.

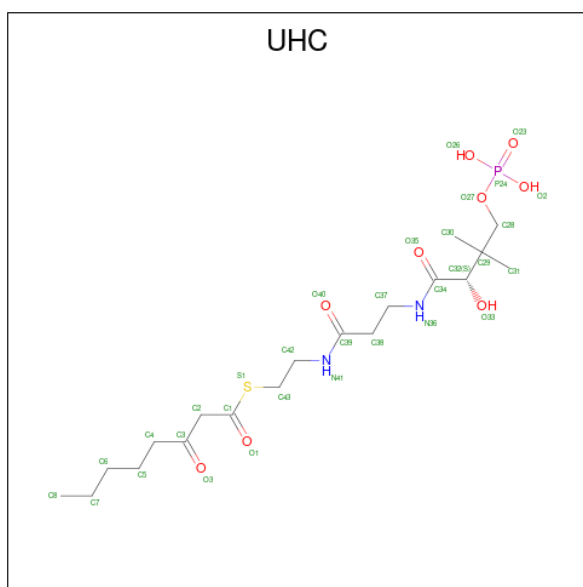
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	73	Total	C	N	O	S	0	0	0
			566	359	85	121	1			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	F	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is {S}-[2-[3-[[2 {S}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] 3-oxidanylideneoctanethioate (CCD ID: UHC) (formula: C₁₉H₃₅N₂O₉PS).

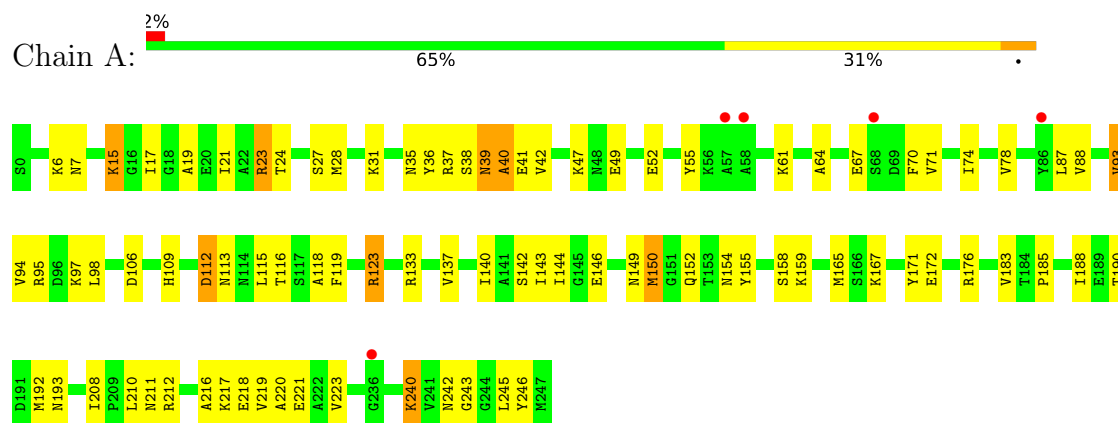


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	S	0	0
			31	19	2	8	1	1		

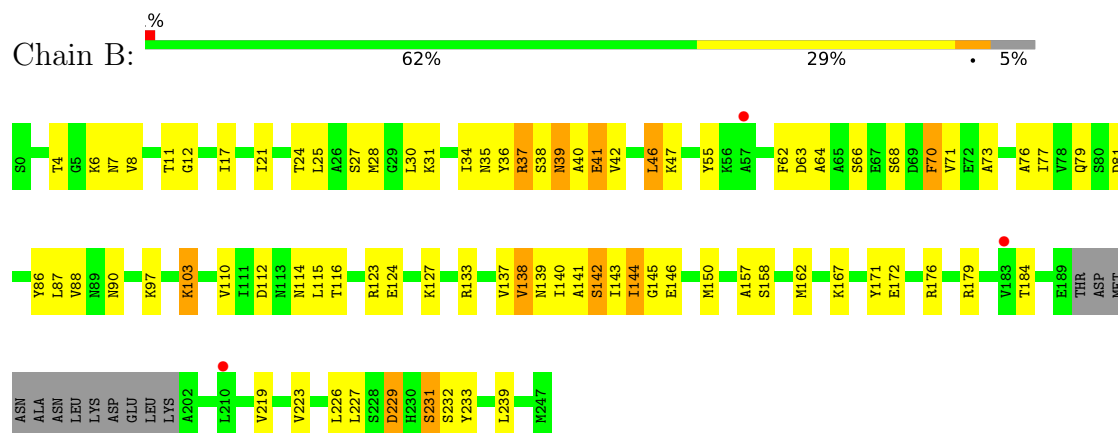
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

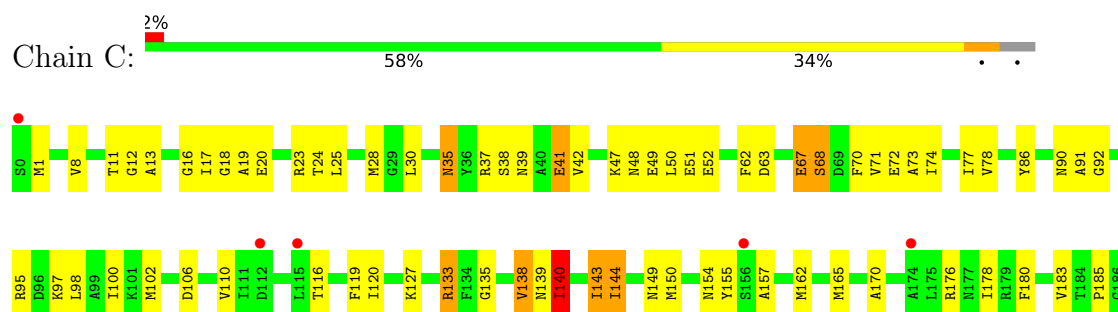
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



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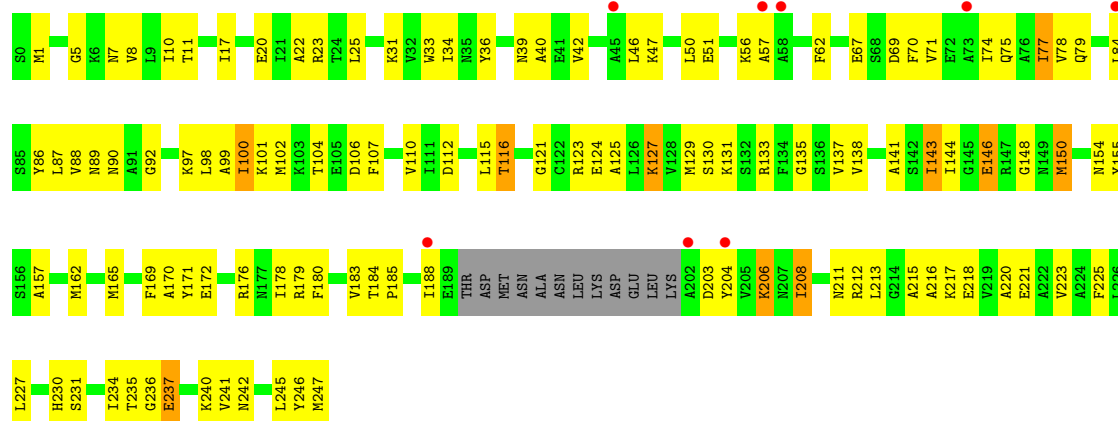


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

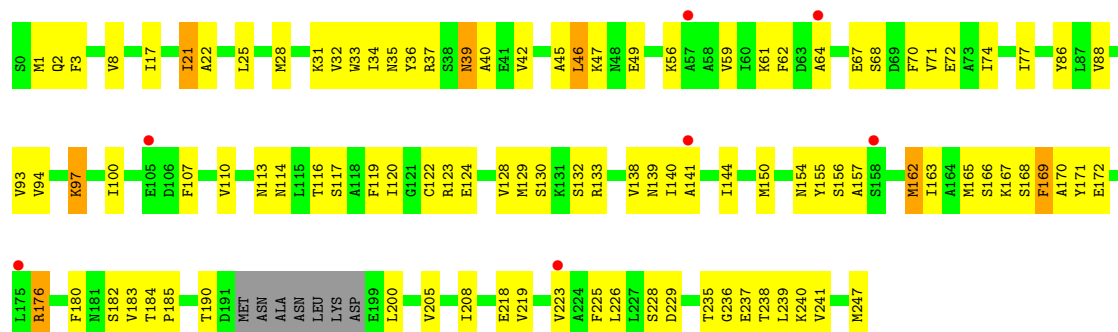




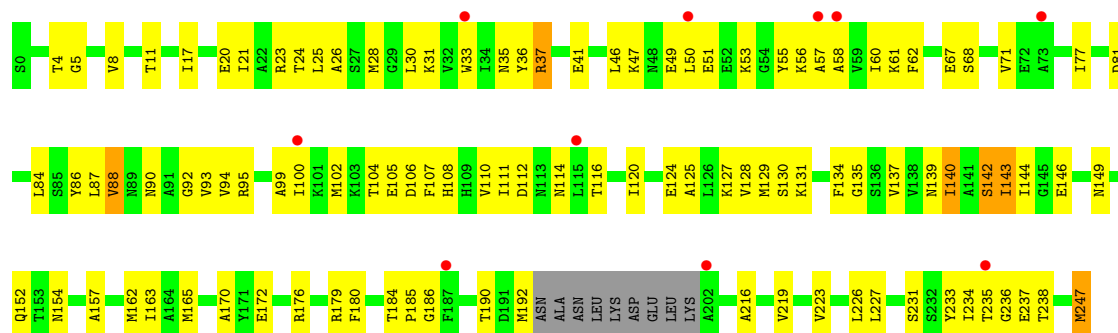
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



• Molecule 2: Acyl carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.42Å 246.93Å 166.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.56 – 2.83 41.56 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.56-2.83) 86.7 (41.56-2.83)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.256 , 0.279 0.257 , 0.278	Depositor DCC
R_{free} test set	1973 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11747	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, UHC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	3/1899 (0.2%)	0.83	7/2553 (0.3%)
1	B	0.78	10/1803 (0.6%)	0.97	4/2423 (0.2%)
1	C	0.67	4/1826 (0.2%)	0.95	8/2454 (0.3%)
1	D	0.57	0/1803	0.95	2/2423 (0.1%)
1	E	0.57	3/1844 (0.2%)	0.89	11/2478 (0.4%)
1	F	0.50	1/1826 (0.1%)	0.77	1/2454 (0.0%)
2	G	0.80	0/571	1.60	13/774 (1.7%)
All	All	0.64	21/11572 (0.2%)	0.94	46/15559 (0.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	SER	C-O	-8.97	1.13	1.24
1	C	138	VAL	C-O	-6.90	1.17	1.24
1	C	140	ILE	C-O	-6.82	1.16	1.23
1	B	139	ASN	C-O	-6.28	1.16	1.24
1	B	66	SER	C-O	-6.22	1.16	1.24
1	B	138	VAL	C-O	-5.72	1.18	1.24
1	B	231	SER	C-O	-5.66	1.16	1.24
1	B	141	ALA	C-O	-5.65	1.16	1.24
1	F	88	VAL	C-O	-5.59	1.18	1.24
1	B	144	ILE	C-O	-5.58	1.17	1.24
1	E	176	ARG	NE-CZ	-5.57	1.26	1.33
1	B	233	TYR	C-O	-5.52	1.17	1.24
1	B	70	PHE	C-O	-5.49	1.17	1.24
1	E	163	ILE	C-O	-5.41	1.18	1.24
1	C	63	ASP	C-O	-5.39	1.17	1.24
1	A	40	ALA	C-O	-5.39	1.16	1.24
1	E	166	SER	C-O	-5.29	1.17	1.24
1	A	240	LYS	C-O	-5.26	1.17	1.24
1	B	142	SER	C-O	-5.18	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	GLU	C-O	-5.00	1.17	1.24
1	B	142	SER	CA-CB	-5.00	1.44	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ARG	CB-CA-C	-9.51	94.35	110.24
1	C	68	SER	CA-C-O	-9.18	111.08	120.90
1	E	176	ARG	CA-C-N	9.04	135.75	122.74
1	E	176	ARG	C-N-CA	9.04	135.75	122.74
1	C	67	GLU	CB-CA-C	-8.91	96.82	110.90
2	G	50	PHE	CA-C-N	-8.63	113.22	120.98
2	G	50	PHE	C-N-CA	-8.63	113.22	120.98
1	E	176	ARG	NE-CZ-NH1	-8.00	113.50	121.50
2	G	51	GLY	N-CA-C	-7.85	98.73	110.97
1	E	176	ARG	CB-CA-C	7.66	123.36	111.02
1	C	190	THR	CB-CA-C	7.63	125.33	109.68
1	B	103	LYS	CB-CG-CD	-7.61	93.79	111.30
2	G	62	ILE	CA-C-O	-6.93	113.16	120.57
2	G	49	LYS	CA-C-N	6.91	132.43	122.40
2	G	49	LYS	C-N-CA	6.91	132.43	122.40
1	A	240	LYS	CB-CA-C	-6.74	99.14	110.19
1	E	46	LEU	CA-C-O	-6.45	113.97	121.07
1	B	233	TYR	N-CA-C	-6.23	105.62	112.72
1	A	37	ARG	CB-CG-CD	6.16	125.46	111.30
1	A	112	ASP	CA-CB-CG	-6.15	106.45	112.60
1	D	206	LYS	CD-CE-NZ	-6.08	92.45	111.90
1	A	37	ARG	CG-CD-NE	5.99	125.17	112.00
2	G	50	PHE	CA-CB-CG	-5.95	107.85	113.80
1	E	21	ILE	N-CA-C	-5.94	104.53	110.30
1	E	176	ARG	NE-CZ-NH2	5.93	124.53	119.20
1	E	176	ARG	CA-CB-CG	5.83	125.77	114.10
2	G	14	GLN	CA-C-N	-5.74	114.23	122.67
2	G	14	GLN	C-N-CA	-5.74	114.23	122.67
2	G	62	ILE	N-CA-C	5.68	116.49	108.36
1	E	37	ARG	N-CA-C	-5.67	107.36	114.56
2	G	51	GLY	CA-C-N	-5.61	113.91	121.66
2	G	51	GLY	C-N-CA	-5.61	113.91	121.66
1	C	133	ARG	CA-CB-CG	5.54	125.18	114.10
1	D	148	GLY	CA-C-O	-5.51	117.58	121.88
1	A	38	SER	CA-C-O	-5.49	116.64	119.77
1	C	190	THR	CA-C-N	5.38	128.35	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	THR	C-N-CA	5.38	128.35	120.71
1	E	169	PHE	CB-CA-C	-5.38	101.86	110.79
1	B	46	LEU	CA-C-O	-5.33	115.22	120.82
1	F	41	GLU	CB-CA-C	5.28	119.06	110.24
1	B	145	GLY	N-CA-C	-5.26	108.79	115.31
1	A	52	GLU	CB-CG-CD	5.25	121.53	112.60
1	E	176	ARG	N-CA-CB	-5.18	102.63	110.92
1	C	67	GLU	N-CA-C	-5.16	105.56	111.14
1	A	23	ARG	CB-CA-C	-5.13	102.82	110.88
2	G	50	PHE	CA-C-O	-5.02	114.59	120.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1875	0	1894	82	0
1	B	1780	0	1798	76	0
1	C	1803	0	1818	109	0
1	D	1780	0	1798	143	0
1	E	1821	0	1839	117	0
1	F	1803	0	1818	100	0
2	G	566	0	553	58	0
3	A	48	0	24	6	0
3	B	48	0	25	7	0
3	C	48	0	25	3	0
3	D	48	0	25	4	0
3	E	48	0	25	3	0
3	F	48	0	25	7	0
4	G	31	0	0	2	0
All	All	11747	0	11667	623	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (623) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:CE2	1:A:40:ALA:HB2	1.57	1.39
1:E:34:ILE:HD13	1:E:46:LEU:HD23	1.24	1.18
1:E:167:LYS:HG2	1:F:247:MET:CE	1.77	1.12
1:E:236:GLY:HA3	1:F:247:MET:SD	1.88	1.12
1:E:167:LYS:HG2	1:F:247:MET:HE3	1.16	1.10
1:D:138:VAL:HG11	1:D:223:VAL:HG13	1.12	1.09
1:E:122:CYS:HB3	1:E:169:PHE:CE2	1.87	1.08
1:B:97:LYS:HZ1	1:C:68:SER:HB2	1.13	1.07
1:D:36:TYR:CE2	1:D:40:ALA:HB2	1.90	1.06
1:E:140:ILE:O	1:E:162:MET:HE1	1.54	1.05
1:B:64:ALA:HB3	3:B:301:NAP:N6A	1.71	1.05
1:D:36:TYR:CE2	1:D:40:ALA:CB	2.42	1.02
1:C:139:ASN:HB3	1:C:162:MET:HE3	1.38	1.01
1:E:122:CYS:CB	1:E:169:PHE:CZ	2.45	1.00
1:D:208:ILE:HD13	1:D:211:ASN:N	1.78	0.99
1:A:36:TYR:CE2	1:A:40:ALA:CB	2.47	0.98
1:A:36:TYR:HE2	1:A:40:ALA:HB2	1.25	0.97
1:D:208:ILE:HD13	1:D:211:ASN:H	1.28	0.97
1:E:169:PHE:HB3	1:E:180:PHE:CD2	1.99	0.97
1:D:138:VAL:CG1	1:D:223:VAL:HG13	1.95	0.96
1:B:37:ARG:HH11	1:B:37:ARG:HB3	1.27	0.95
1:B:97:LYS:NZ	1:C:68:SER:HB2	1.81	0.95
1:C:1:MET:HE1	1:C:225:PHE:HA	1.49	0.94
1:D:183:VAL:HG21	1:D:223:VAL:HG22	1.48	0.94
1:E:122:CYS:HB3	1:E:169:PHE:CZ	2.03	0.94
1:C:240:LYS:HG2	1:D:237:GLU:CG	1.98	0.92
1:C:139:ASN:HB3	1:C:162:MET:CE	1.99	0.92
1:D:138:VAL:HG11	1:D:223:VAL:CG1	1.99	0.92
1:E:122:CYS:HB2	1:E:169:PHE:CZ	2.05	0.91
1:B:37:ARG:HB3	1:B:37:ARG:NH1	1.85	0.90
1:D:110:VAL:HG21	1:D:154:ASN:HB2	1.54	0.87
1:D:1:MET:HE1	1:D:225:PHE:HA	1.57	0.86
1:C:41:GLU:N	1:C:41:GLU:OE1	2.09	0.86
1:F:139:ASN:HB3	1:F:162:MET:HE2	1.57	0.85
1:D:127:LYS:HD3	1:E:100:ILE:HG22	1.60	0.84
1:F:142:SER:HB2	3:F:301:NAP:H6N	1.59	0.84
1:E:74:ILE:O	1:E:77:ILE:HG22	1.78	0.83
1:F:86:TYR:HB3	1:F:227:LEU:HD23	1.60	0.83
1:E:34:ILE:CD1	1:E:46:LEU:HD23	2.08	0.82
2:G:57:GLU:O	2:G:61:LYS:HG3	1.80	0.82
2:G:58:GLN:HG2	2:G:71:TYR:CD1	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:GLY:HA3	3:C:301:NAP:H3D	1.64	0.80
1:C:187:PHE:HE2	1:C:204:TYR:HE2	1.29	0.80
1:D:77:ILE:HG21	1:D:84:LEU:HB2	1.62	0.79
1:A:36:TYR:CD2	1:A:40:ALA:HB2	2.18	0.79
1:B:64:ALA:HB3	3:B:301:NAP:C6A	2.12	0.78
1:C:240:LYS:HG2	1:D:237:GLU:CD	2.08	0.78
1:E:21:ILE:HG22	1:E:25:LEU:HD21	1.64	0.78
1:B:97:LYS:NZ	1:C:68:SER:CB	2.47	0.77
1:F:129:MET:HE3	1:F:135:GLY:HA3	1.67	0.77
1:B:34:ILE:HD13	1:B:46:LEU:HD23	1.67	0.77
1:A:95:ARG:NH1	1:A:109:HIS:ND1	2.33	0.77
1:A:109:HIS:HD2	1:A:113:ASN:HD22	1.31	0.77
1:B:62:PHE:CD2	1:B:70:PHE:HA	2.20	0.77
1:D:17:ILE:HD11	1:D:188:ILE:HG13	1.64	0.76
1:B:140:ILE:O	1:B:162:MET:HE1	1.85	0.76
1:D:208:ILE:CD1	1:D:212:ARG:H	1.98	0.76
1:F:35:ASN:OD1	1:F:62:PHE:CE2	2.38	0.76
1:B:133:ARG:HH11	1:B:176:ARG:HG3	1.50	0.76
1:C:240:LYS:CG	1:D:237:GLU:CG	2.62	0.76
1:C:233:TYR:HB2	1:D:218:GLU:OE1	1.86	0.76
1:A:183:VAL:HG12	1:A:185:PRO:HD3	1.67	0.76
1:D:36:TYR:CE2	1:D:40:ALA:HB1	2.19	0.75
1:B:90:ASN:OD1	3:B:301:NAP:H4D	1.87	0.75
1:F:35:ASN:OD1	1:F:62:PHE:CZ	2.40	0.75
1:D:74:ILE:O	1:D:77:ILE:HB	1.86	0.75
1:E:141:ALA:HB3	1:E:184:THR:HG22	1.69	0.74
1:E:122:CYS:CB	1:E:169:PHE:CE2	2.65	0.74
1:B:179:ARG:NH2	1:B:226:LEU:O	2.21	0.74
1:D:203:ASP:C	1:D:206:LYS:HZ1	1.95	0.74
1:F:110:VAL:HG21	1:F:154:ASN:HD22	1.51	0.74
1:E:240:LYS:HB2	1:F:237:GLU:HG3	1.70	0.74
1:F:149:ASN:HD22	1:F:152:GLN:HE21	1.34	0.73
1:A:39:ASN:OD1	1:A:39:ASN:N	2.21	0.73
1:E:1:MET:HE1	1:E:225:PHE:HA	1.72	0.72
1:B:37:ARG:HD3	1:B:63:ASP:CG	2.14	0.72
1:C:110:VAL:HG21	1:C:154:ASN:HD22	1.54	0.72
2:G:11:ILE:HG12	2:G:42:LEU:HD11	1.72	0.72
1:F:231:SER:HA	1:F:234:ILE:HD12	1.72	0.71
1:C:188:ILE:HG22	1:C:190:THR:H	1.54	0.71
1:C:25:LEU:HD12	1:C:30:LEU:HD12	1.73	0.71
1:B:140:ILE:O	1:B:162:MET:CE	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLU:HA	1:C:120:ILE:HD13	1.73	0.70
1:D:87:LEU:HD21	1:D:89:ASN:ND2	2.04	0.70
1:D:36:TYR:HE2	1:D:40:ALA:HB1	1.55	0.70
1:C:133:ARG:HH11	1:C:176:ARG:HG2	1.57	0.70
1:E:21:ILE:HG22	1:E:25:LEU:CD2	2.21	0.70
1:F:17:ILE:O	1:F:21:ILE:HG13	1.91	0.70
1:B:86:TYR:HB3	1:B:227:LEU:HD22	1.72	0.69
2:G:12:ALA:HA	2:G:17:VAL:HG23	1.74	0.69
2:G:57:GLU:CD	2:G:57:GLU:H	2.00	0.69
1:C:98:LEU:HD22	1:C:100:ILE:HG12	1.74	0.69
1:C:240:LYS:HG2	1:D:237:GLU:OE2	1.91	0.69
1:A:143:ILE:HD13	1:A:245:LEU:HD23	1.73	0.69
1:D:179:ARG:HA	1:D:235:THR:HG22	1.75	0.69
3:F:301:NAP:H2N	3:F:301:NAP:H51N	1.75	0.68
1:D:98:LEU:HD22	1:D:100:ILE:HG12	1.76	0.68
1:C:150:MET:HG3	1:F:172:GLU:HG2	1.76	0.68
1:B:39:ASN:N	1:B:39:ASN:OD1	2.27	0.68
1:E:133:ARG:CZ	1:E:176:ARG:NH1	2.57	0.67
1:E:122:CYS:HB3	1:E:169:PHE:CD2	2.30	0.67
1:E:140:ILE:O	1:E:162:MET:CE	2.38	0.67
2:G:58:GLN:CG	2:G:71:TYR:CD1	2.77	0.67
1:A:15:LYS:HE2	3:A:301:NAP:H3B	1.74	0.67
1:E:205:VAL:HA	1:E:208:ILE:HD12	1.75	0.67
2:G:52:ILE:C	2:G:52:ILE:HD12	2.19	0.67
1:E:167:LYS:CG	1:F:247:MET:CE	2.64	0.67
1:A:192:MET:HE1	3:A:301:NAP:H2D	1.75	0.67
2:G:27:GLU:O	2:G:31:ASP:HB2	1.95	0.67
1:F:163:ILE:HG23	1:F:238:THR:HG21	1.75	0.67
1:A:87:LEU:HB3	1:A:137:VAL:HG13	1.76	0.67
1:F:99:ALA:HA	1:F:102:MET:HE2	1.77	0.67
1:C:240:LYS:HG2	1:D:237:GLU:HG3	1.77	0.66
1:A:17:ILE:O	1:A:21:ILE:HD12	1.95	0.66
1:A:36:TYR:CE1	1:A:61:LYS:HB2	2.30	0.66
1:B:68:SER:HB2	1:C:97:LYS:HE2	1.78	0.66
1:B:64:ALA:HB3	3:B:301:NAP:H62A	1.59	0.66
1:D:75:GLN:OE1	1:D:79:GLN:HG2	1.96	0.66
1:A:133:ARG:HH11	1:A:176:ARG:HG3	1.60	0.66
1:B:62:PHE:HD2	1:B:70:PHE:HA	1.61	0.65
1:F:223:VAL:HG12	1:F:227:LEU:HD11	1.79	0.65
2:G:53:GLU:O	2:G:54:ILE:C	2.38	0.65
1:D:204:TYR:N	1:D:206:LYS:HZ1	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:GLU:HG2	1:E:150:MET:HG3	1.78	0.65
1:E:133:ARG:CZ	1:E:176:ARG:HH12	2.09	0.65
1:F:219:VAL:O	1:F:223:VAL:HG23	1.97	0.65
1:A:109:HIS:CD2	1:A:113:ASN:HD22	2.14	0.65
1:B:144:ILE:HD13	1:B:144:ILE:N	2.11	0.65
1:C:12:GLY:H	1:C:35:ASN:ND2	1.95	0.65
1:C:240:LYS:CG	1:D:237:GLU:HG3	2.26	0.65
1:D:87:LEU:HB3	1:D:137:VAL:HG22	1.79	0.65
1:C:23:ARG:NH1	1:C:49:GLU:OE2	2.29	0.65
1:D:17:ILE:HB	3:D:301:NAP:H51N	1.77	0.64
1:D:46:LEU:HD23	1:D:46:LEU:C	2.22	0.64
1:F:90:ASN:OD1	3:F:301:NAP:H4D	1.97	0.64
1:F:140:ILE:HD13	1:F:140:ILE:N	2.11	0.64
2:G:58:GLN:OE1	2:G:71:TYR:HB3	1.97	0.64
1:C:23:ARG:HG2	1:C:50:LEU:HD11	1.79	0.64
1:D:62:PHE:HB2	1:D:69:ASP:HB3	1.79	0.64
1:F:149:ASN:HD22	1:F:152:GLN:NE2	1.95	0.64
1:F:4:THR:HB	1:F:134:PHE:HZ	1.62	0.64
1:E:169:PHE:CD2	1:E:180:PHE:CZ	2.86	0.64
1:A:165:MET:HB3	1:B:157:ALA:HB2	1.79	0.64
1:B:229:ASP:OD1	1:B:229:ASP:N	2.30	0.64
1:C:133:ARG:NH1	1:C:176:ARG:HG2	2.12	0.64
1:B:64:ALA:HB2	3:B:301:NAP:N1A	2.13	0.64
1:F:87:LEU:HB3	1:F:137:VAL:HG22	1.80	0.64
1:E:169:PHE:HD2	1:E:180:PHE:CZ	2.16	0.63
1:F:47:LYS:HD3	1:F:51:GLU:OE2	1.99	0.63
1:D:74:ILE:HD13	1:D:124:GLU:HB3	1.80	0.63
1:D:112:ASP:HA	1:D:116:THR:CG2	2.28	0.63
1:D:150:MET:HG2	1:E:172:GLU:HG2	1.79	0.63
1:E:167:LYS:CG	1:F:247:MET:HE3	2.11	0.63
1:C:74:ILE:O	1:C:78:VAL:HG23	1.97	0.63
1:A:17:ILE:HA	1:A:216:ALA:HB1	1.81	0.63
1:A:208:ILE:HG13	1:A:245:LEU:HD13	1.78	0.63
1:D:208:ILE:HD13	1:D:212:ARG:H	1.62	0.63
1:C:157:ALA:HB2	1:F:165:MET:HB2	1.81	0.63
1:C:110:VAL:HG21	1:C:154:ASN:ND2	2.13	0.63
1:D:155:TYR:OH	3:D:301:NAP:H2N	1.98	0.63
1:E:74:ILE:HA	1:E:77:ILE:HG22	1.79	0.63
1:C:11:THR:HG22	1:C:91:ALA:HB2	1.81	0.62
1:E:122:CYS:C	1:E:169:PHE:CE2	2.77	0.62
1:F:110:VAL:HG21	1:F:154:ASN:ND2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:SER:HB2	3:F:301:NAP:C6N	2.30	0.62
1:F:179:ARG:NH2	1:F:231:SER:OG	2.32	0.62
1:B:123:ARG:HG2	1:B:127:LYS:HE2	1.81	0.62
1:B:138:VAL:HG11	1:B:223:VAL:HG13	1.81	0.62
1:C:72:GLU:OE1	1:C:72:GLU:N	2.31	0.62
1:C:11:THR:O	1:C:90:ASN:HB3	1.99	0.62
1:F:127:LYS:HD2	1:F:131:LYS:NZ	2.14	0.62
1:F:223:VAL:O	1:F:227:LEU:HD12	1.99	0.62
1:F:4:THR:HB	1:F:134:PHE:CZ	2.35	0.61
1:F:36:TYR:O	1:F:61:LYS:HA	2.00	0.61
1:A:149:ASN:HB3	1:A:152:GLN:HG3	1.81	0.61
1:B:64:ALA:CB	3:B:301:NAP:C6A	2.79	0.61
1:E:93:VAL:HG22	1:E:94:VAL:H	1.65	0.61
2:G:48:GLU:HG3	2:G:48:GLU:O	2.00	0.61
2:G:53:GLU:O	2:G:55:PRO:N	2.33	0.61
1:A:97:LYS:HE3	1:A:106:ASP:OD2	2.01	0.61
1:B:62:PHE:HE2	1:B:70:PHE:CG	2.19	0.61
2:G:64:ASN:ND2	2:G:67:ASP:OD2	2.28	0.60
1:D:110:VAL:CG2	1:D:154:ASN:HB2	2.31	0.60
1:F:137:VAL:HB	1:F:180:PHE:CD1	2.35	0.60
1:C:8:VAL:HG23	1:C:86:TYR:HB2	1.83	0.60
1:D:97:LYS:NZ	1:D:102:MET:HA	2.17	0.60
1:B:62:PHE:CE2	1:B:70:PHE:HA	2.37	0.60
1:C:102:MET:HE1	1:C:154:ASN:OD1	2.02	0.60
1:E:167:LYS:HA	1:F:247:MET:HE1	1.84	0.60
1:E:171:TYR:HD1	1:E:171:TYR:N	2.00	0.60
1:B:24:THR:HG22	1:B:28:MET:HE3	1.83	0.59
2:G:28:PHE:CE1	2:G:65:VAL:HG12	2.36	0.59
1:E:62:PHE:HE2	1:E:70:PHE:CD1	2.19	0.59
1:C:12:GLY:H	1:C:35:ASN:HD22	1.48	0.59
1:E:141:ALA:O	3:E:301:NAP:H6N	2.03	0.59
1:E:169:PHE:HB3	1:E:180:PHE:CG	2.37	0.59
1:F:170:ALA:HB1	1:F:235:THR:HG22	1.85	0.59
1:C:240:LYS:CG	1:D:237:GLU:HG2	2.33	0.59
1:D:183:VAL:O	1:D:185:PRO:HD3	2.04	0.58
2:G:6:ASP:O	2:G:10:VAL:HG23	2.03	0.58
1:A:115:LEU:HD12	1:A:158:SER:HA	1.83	0.58
1:E:183:VAL:HG12	1:E:185:PRO:HD3	1.86	0.58
1:B:115:LEU:HD12	1:B:158:SER:HA	1.86	0.58
1:E:219:VAL:O	1:E:223:VAL:HG23	2.02	0.58
2:G:39:VAL:O	2:G:43:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD13	1:D:125:ALA:HB2	1.84	0.58
1:D:127:LYS:HD3	1:E:100:ILE:CG2	2.32	0.58
2:G:12:ALA:HB1	2:G:17:VAL:O	2.04	0.58
2:G:52:ILE:HD12	2:G:53:GLU:N	2.18	0.58
1:D:141:ALA:HA	1:D:162:MET:HE1	1.86	0.57
1:F:77:ILE:HG21	1:F:84:LEU:HD12	1.85	0.57
1:C:86:TYR:HB3	1:C:227:LEU:HD22	1.85	0.57
1:C:187:PHE:HE2	1:C:204:TYR:CE2	2.16	0.57
1:B:64:ALA:CB	3:B:301:NAP:N1A	2.68	0.57
1:E:169:PHE:HB3	1:E:180:PHE:CE2	2.40	0.57
1:E:171:TYR:N	1:E:171:TYR:CD1	2.73	0.57
1:A:155:TYR:HE1	1:A:159:LYS:HE2	1.69	0.57
1:A:36:TYR:CZ	1:A:61:LYS:HB2	2.40	0.57
1:D:143:ILE:HD11	1:D:246:TYR:HB2	1.86	0.57
1:D:206:LYS:HD3	1:D:206:LYS:N	2.20	0.57
1:E:39:ASN:HD21	1:E:42:VAL:HG22	1.69	0.57
2:G:36:SER:O	2:G:39:VAL:N	2.38	0.57
1:D:131:LYS:HA	1:D:133:ARG:NH1	2.20	0.57
2:G:58:GLN:HG2	2:G:71:TYR:CE1	2.39	0.57
1:D:146:GLU:OE1	1:D:184:THR:HG21	2.05	0.57
1:D:33:TRP:CH2	1:D:77:ILE:HA	2.40	0.56
1:D:77:ILE:HG22	1:D:78:VAL:N	2.20	0.56
2:G:35:ASP:N	2:G:38:ASP:OD2	2.37	0.56
1:A:19:ALA:O	1:A:23:ARG:HG3	2.05	0.56
1:B:25:LEU:HD12	1:B:30:LEU:HD12	1.86	0.56
1:C:143:ILE:HG23	1:C:185:PRO:O	2.05	0.56
1:F:143:ILE:HG12	1:F:186:GLY:HA2	1.87	0.56
2:G:62:ILE:O	2:G:62:ILE:HG22	2.05	0.56
1:C:35:ASN:HD21	3:C:301:NAP:H2A	1.71	0.56
1:D:208:ILE:HD12	1:D:212:ARG:H	1.70	0.56
1:D:115:LEU:HD22	1:E:107:PHE:CZ	2.41	0.56
1:C:237:GLU:HG3	1:D:240:LYS:HB2	1.88	0.56
1:D:138:VAL:CB	1:D:223:VAL:CG1	2.84	0.56
1:E:169:PHE:HD2	1:E:180:PHE:CE2	2.23	0.56
1:C:230:HIS:HA	1:D:221:GLU:OE1	2.05	0.56
1:C:70:PHE:HD1	1:C:70:PHE:O	1.89	0.56
1:D:100:ILE:HG13	1:D:101:LYS:N	2.21	0.55
1:F:130:SER:HB3	1:F:176:ARG:HD2	1.88	0.55
1:A:155:TYR:CE1	1:A:159:LYS:HE2	2.41	0.55
1:D:137:VAL:HB	1:D:180:PHE:CD1	2.41	0.55
1:D:138:VAL:CG1	1:D:223:VAL:CG1	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ASN:OD1	1:D:245:LEU:N	2.40	0.55
1:B:167:LYS:O	1:B:171:TYR:HD1	1.90	0.55
1:C:48:ASN:O	1:C:52:GLU:HG3	2.06	0.55
1:B:176:ARG:CD	2:G:37:LEU:HD11	2.37	0.55
1:C:236:GLY:HA3	1:D:247:MET:SD	2.47	0.55
1:F:31:LYS:NZ	1:F:81:ASP:OD1	2.37	0.55
1:A:217:LYS:O	1:A:221:GLU:HG3	2.07	0.55
1:B:97:LYS:HZ3	1:C:68:SER:CB	2.19	0.55
1:B:142:SER:O	1:B:184:THR:HB	2.07	0.55
1:E:62:PHE:CE2	1:E:70:PHE:CD1	2.94	0.55
1:F:47:LYS:O	1:F:51:GLU:HG3	2.07	0.55
1:F:223:VAL:HG12	1:F:227:LEU:CD1	2.37	0.55
1:A:119:PHE:N	1:A:165:MET:HE1	2.22	0.54
1:D:176:ARG:HB2	1:D:178:ILE:CD1	2.37	0.54
1:A:143:ILE:HD11	1:A:246:TYR:HB2	1.89	0.54
1:B:73:ALA:O	1:B:77:ILE:HD12	2.07	0.54
1:C:170:ALA:HB2	1:C:180:PHE:HB2	1.89	0.54
1:C:140:ILE:O	1:C:162:MET:HE1	2.07	0.54
1:F:95:ARG:NH2	1:F:106:ASP:OD1	2.39	0.54
2:G:29:VAL:HA	2:G:34:ALA:H	1.71	0.54
1:F:21:ILE:O	1:F:25:LEU:HG	2.07	0.54
1:A:152:GLN:HE22	4:G:101:UHC:C43	2.20	0.54
1:B:17:ILE:O	1:B:21:ILE:HD12	2.07	0.54
1:B:176:ARG:CZ	2:G:37:LEU:HD21	2.37	0.54
1:C:230:HIS:HB3	1:D:221:GLU:HB3	1.88	0.54
1:D:87:LEU:HD22	1:D:137:VAL:HG13	1.90	0.54
1:D:112:ASP:HA	1:D:116:THR:HG21	1.89	0.54
1:A:61:LYS:O	1:A:61:LYS:HG2	2.08	0.54
1:C:187:PHE:CE2	1:C:204:TYR:HE2	2.18	0.54
1:F:46:LEU:O	1:F:50:LEU:HG	2.07	0.53
1:B:79:GLN:O	1:B:79:GLN:HG3	2.07	0.53
1:D:115:LEU:HD22	1:E:107:PHE:HZ	1.74	0.53
1:E:64:ALA:HB1	1:E:117:SER:HB2	1.89	0.53
1:D:112:ASP:HA	1:D:116:THR:HG23	1.90	0.53
1:D:169:PHE:HB3	1:D:180:PHE:CD2	2.43	0.53
1:D:185:PRO:HB2	3:D:301:NAP:H5N	1.89	0.53
1:E:138:VAL:HG21	1:E:223:VAL:HG13	1.91	0.53
1:B:144:ILE:C	1:B:146:GLU:H	2.17	0.53
1:F:8:VAL:HA	1:F:86:TYR:O	2.08	0.53
1:B:176:ARG:NE	2:G:37:LEU:HD11	2.24	0.53
1:C:73:ALA:O	1:C:77:ILE:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:46:LEU:N	2:G:46:LEU:CD1	2.72	0.53
1:B:73:ALA:O	1:B:76:ALA:N	2.42	0.53
1:D:34:ILE:HD11	1:D:57:ALA:HB1	1.91	0.53
1:C:247:MET:CE	1:D:236:GLY:HA3	2.39	0.52
1:F:37:ARG:HG3	3:F:301:NAP:C2A	2.39	0.52
1:D:180:PHE:O	1:D:236:GLY:N	2.32	0.52
1:A:35:ASN:HD21	3:A:301:NAP:H2A	1.75	0.52
1:D:102:MET:O	1:E:123:ARG:NH1	2.35	0.52
2:G:56:ASP:O	2:G:59:ALA:N	2.42	0.52
1:A:109:HIS:CD2	1:A:113:ASN:ND2	2.77	0.52
1:A:143:ILE:HG23	1:A:144:ILE:HD12	1.91	0.52
1:F:87:LEU:HD13	1:F:125:ALA:HB2	1.91	0.52
1:D:36:TYR:CZ	1:D:40:ALA:HB2	2.43	0.52
1:E:39:ASN:ND2	1:E:42:VAL:HG22	2.25	0.52
1:E:31:LYS:HG3	1:E:56:LYS:HB3	1.90	0.52
1:E:110:VAL:O	1:E:114:ASN:HB2	2.09	0.52
1:F:36:TYR:CZ	1:F:61:LYS:HB2	2.44	0.52
1:A:109:HIS:HD2	1:A:113:ASN:ND2	2.02	0.52
1:C:67:GLU:HB2	1:F:104:THR:HG21	1.92	0.52
1:F:139:ASN:HB3	1:F:162:MET:CE	2.34	0.52
2:G:15:LEU:O	2:G:15:LEU:HD12	2.10	0.52
1:A:7:ASN:HB3	1:A:31:LYS:CG	2.41	0.51
1:C:237:GLU:OE2	1:D:240:LYS:HE3	2.10	0.51
1:D:36:TYR:CD2	1:D:40:ALA:CB	2.93	0.51
1:B:25:LEU:CD1	1:B:30:LEU:HD12	2.40	0.51
1:E:46:LEU:O	1:E:49:GLU:HB2	2.11	0.51
1:A:208:ILE:HG12	1:A:245:LEU:HB2	1.92	0.51
1:D:106:ASP:O	1:D:110:VAL:HG22	2.10	0.51
1:E:68:SER:O	1:E:72:GLU:HG3	2.11	0.51
2:G:36:SER:O	2:G:37:LEU:C	2.54	0.51
1:A:93:VAL:HG23	1:A:113:ASN:HB3	1.92	0.51
1:A:95:ARG:CZ	1:A:109:HIS:ND1	2.74	0.51
1:C:13:ALA:HA	1:C:18:GLY:HA3	1.92	0.51
1:C:127:LYS:HG3	1:F:100:ILE:HG22	1.92	0.51
1:C:240:LYS:HD3	1:C:242:ASN:HD21	1.75	0.51
1:D:67:GLU:O	1:D:71:VAL:HG23	2.11	0.51
1:A:167:LYS:O	1:A:171:TYR:HD1	1.94	0.50
1:C:240:LYS:HG3	1:D:237:GLU:HG3	1.93	0.50
1:D:123:ARG:O	1:D:127:LYS:HG2	2.11	0.50
1:E:35:ASN:OD1	1:E:36:TYR:N	2.44	0.50
1:E:122:CYS:CB	1:E:169:PHE:CE1	2.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:35:ASP:OD1	2:G:36:SER:N	2.44	0.50
1:C:140:ILE:N	1:C:140:ILE:HD13	2.25	0.50
1:A:112:ASP:HA	1:A:116:THR:OG1	2.11	0.50
1:C:165:MET:HB2	1:F:157:ALA:HB2	1.93	0.50
1:D:70:PHE:CE1	1:D:121:GLY:HA2	2.46	0.50
1:E:124:GLU:O	1:E:128:VAL:HG12	2.11	0.50
1:A:193:ASN:ND2	4:G:101:UHC:S1	2.84	0.50
1:D:20:GLU:HG3	1:D:216:ALA:HB3	1.93	0.50
1:E:36:TYR:CZ	1:E:61:LYS:HB2	2.47	0.50
1:E:122:CYS:HB2	1:E:169:PHE:CE1	2.45	0.50
1:B:143:ILE:HG23	1:B:144:ILE:HD13	1.94	0.50
1:D:92:GLY:O	3:D:301:NAP:H52A	2.12	0.50
1:E:33:TRP:CE2	1:E:77:ILE:HD11	2.47	0.50
1:E:218:GLU:OE1	1:F:233:TYR:HB2	2.12	0.50
1:F:67:GLU:O	1:F:71:VAL:HG12	2.12	0.50
1:D:217:LYS:HA	1:D:220:ALA:HB3	1.94	0.50
1:E:170:ALA:HB1	1:E:235:THR:OG1	2.11	0.50
2:G:57:GLU:CD	2:G:57:GLU:N	2.70	0.50
1:C:1:MET:HE1	1:C:225:PHE:CA	2.31	0.50
1:E:122:CYS:O	1:E:169:PHE:HE2	1.95	0.50
1:F:143:ILE:HG23	1:F:185:PRO:O	2.12	0.50
1:B:176:ARG:NH1	2:G:37:LEU:HD21	2.27	0.49
1:C:16:GLY:HA2	1:C:190:THR:HG21	1.93	0.49
1:D:129:MET:SD	1:D:135:GLY:HA3	2.52	0.49
1:E:22:ALA:HB1	1:E:32:VAL:HG11	1.94	0.49
1:E:144:ILE:HG22	1:E:156:SER:HB3	1.92	0.49
1:F:93:VAL:HG12	1:F:114:ASN:OD1	2.13	0.49
1:D:11:THR:O	1:D:90:ASN:HB3	2.12	0.49
1:A:17:ILE:HG22	1:A:21:ILE:HD11	1.94	0.49
1:D:146:GLU:CD	1:D:184:THR:HG21	2.37	0.49
1:C:19:ALA:O	1:C:23:ARG:HG3	2.12	0.49
1:A:7:ASN:HB3	1:A:31:LYS:HG3	1.93	0.49
1:A:17:ILE:HG13	1:A:190:THR:HG21	1.95	0.49
1:C:217:LYS:HG2	1:C:221:GLU:OE2	2.12	0.49
1:D:203:ASP:HA	1:D:206:LYS:NZ	2.27	0.49
1:E:247:MET:SD	1:F:236:GLY:HA3	2.53	0.49
1:E:17:ILE:O	1:E:21:ILE:HG13	2.12	0.49
1:C:183:VAL:O	1:C:185:PRO:HD3	2.13	0.49
1:D:208:ILE:HD12	1:D:212:ARG:O	2.13	0.49
1:C:241:VAL:HG22	1:D:234:ILE:HD11	1.95	0.49
1:E:34:ILE:HD13	1:E:46:LEU:CD2	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:O	1:B:162:MET:HE3	2.13	0.48
1:D:137:VAL:HB	1:D:180:PHE:HD1	1.77	0.48
1:E:167:LYS:HG2	1:F:247:MET:HE1	1.85	0.48
1:E:200:LEU:HD23	1:E:200:LEU:H	1.78	0.48
1:C:247:MET:SD	1:D:171:TYR:HE1	2.37	0.48
1:F:170:ALA:HA	1:F:180:PHE:HD2	1.78	0.48
1:B:34:ILE:CD1	1:B:46:LEU:HD23	2.42	0.48
1:C:35:ASN:HB2	1:C:62:PHE:CE1	2.48	0.48
1:D:47:LYS:HE3	1:D:51:GLU:OE2	2.13	0.48
1:B:47:LYS:C	1:B:47:LYS:HD2	2.37	0.48
1:D:5:GLY:HA3	1:D:86:TYR:CE2	2.49	0.48
1:B:144:ILE:C	1:B:146:GLU:N	2.71	0.48
1:C:149:ASN:OD1	1:C:150:MET:N	2.45	0.48
1:B:110:VAL:O	1:B:114:ASN:HB2	2.13	0.48
1:E:61:LYS:O	1:E:62:PHE:HB3	2.14	0.48
1:E:226:LEU:HD11	1:E:239:LEU:HD12	1.95	0.48
1:A:119:PHE:HA	1:A:165:MET:HE1	1.95	0.48
1:D:36:TYR:CD2	1:D:40:ALA:HB2	2.44	0.48
1:F:127:LYS:HD2	1:F:131:LYS:HZ3	1.79	0.48
1:B:12:GLY:H	1:B:35:ASN:ND2	2.11	0.47
1:E:133:ARG:NH1	1:E:176:ARG:NH1	2.61	0.47
1:A:64:ALA:HA	1:A:70:PHE:HD2	1.79	0.47
1:B:12:GLY:H	1:B:35:ASN:HD22	1.62	0.47
1:B:41:GLU:N	1:B:41:GLU:OE1	2.48	0.47
1:A:7:ASN:HB3	1:A:31:LYS:HD2	1.96	0.47
1:B:17:ILE:CG2	1:B:21:ILE:HD11	2.45	0.47
1:D:138:VAL:HG21	1:D:223:VAL:CG1	2.44	0.47
1:E:47:LYS:HD2	1:E:59:VAL:HG23	1.97	0.47
1:E:141:ALA:CB	1:E:184:THR:HG22	2.42	0.47
2:G:14:GLN:O	2:G:14:GLN:HG3	2.14	0.47
2:G:37:LEU:HD23	2:G:38:ASP:N	2.29	0.47
1:A:133:ARG:NH1	1:A:176:ARG:HG3	2.28	0.47
1:C:20:GLU:HG3	1:C:216:ALA:HB3	1.95	0.47
1:D:138:VAL:CB	1:D:223:VAL:HG13	2.42	0.47
1:D:141:ALA:HB3	1:D:184:THR:HA	1.97	0.47
1:A:210:LEU:HD12	1:A:243:GLY:HA2	1.96	0.47
1:D:144:ILE:N	1:D:144:ILE:HD13	2.28	0.47
1:A:6:LYS:O	1:A:31:LYS:HG2	2.14	0.47
1:A:154:ASN:OD1	1:A:155:TYR:N	2.45	0.47
1:C:247:MET:HE1	1:D:170:ALA:HB3	1.97	0.47
1:D:71:VAL:O	1:D:74:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:LYS:HZ1	1:D:102:MET:HA	1.80	0.47
1:A:188:ILE:HG22	1:A:190:THR:HG23	1.97	0.47
1:C:35:ASN:ND2	1:C:35:ASN:C	2.73	0.47
1:E:116:THR:O	1:E:120:ILE:HG13	2.15	0.47
1:A:152:GLN:OE1	1:A:155:TYR:HD2	1.97	0.47
1:E:138:VAL:C	1:E:139:ASN:HD22	2.23	0.47
1:A:242:ASN:OD1	1:A:245:LEU:N	2.48	0.47
1:E:74:ILE:CA	1:E:77:ILE:HG22	2.43	0.47
1:E:97:LYS:HD3	1:E:97:LYS:HA	1.52	0.47
1:E:190:THR:HB	3:E:301:NAP:H72N	1.80	0.47
1:E:237:GLU:CD	1:E:238:THR:H	2.23	0.47
1:F:49:GLU:O	1:F:53:LYS:HG2	2.15	0.47
1:A:192:MET:CE	3:A:301:NAP:H2D	2.42	0.46
1:A:212:ARG:NH2	1:A:218:GLU:OE2	2.45	0.46
1:D:138:VAL:HB	1:D:223:VAL:CG1	2.45	0.46
1:F:33:TRP:CD2	1:F:77:ILE:HD11	2.50	0.46
1:A:36:TYR:CD2	1:A:40:ALA:CB	2.89	0.46
1:C:188:ILE:C	1:C:190:THR:N	2.70	0.46
1:C:138:VAL:HG23	1:C:227:LEU:CD2	2.46	0.46
1:E:39:ASN:HD21	1:E:42:VAL:HG13	1.81	0.46
1:C:234:ILE:HG12	1:D:241:VAL:HG22	1.97	0.46
1:D:31:LYS:HG3	1:D:56:LYS:HB3	1.96	0.46
1:D:131:LYS:O	1:D:133:ARG:NH1	2.46	0.46
1:A:119:PHE:CA	1:A:165:MET:HE1	2.44	0.46
1:D:46:LEU:HD21	1:D:50:LEU:HD11	1.97	0.46
1:F:5:GLY:HA3	1:F:86:TYR:CE2	2.50	0.46
2:G:52:ILE:C	2:G:52:ILE:CD1	2.85	0.46
1:F:127:LYS:HD2	1:F:131:LYS:HZ1	1.80	0.46
1:D:102:MET:HG3	1:E:119:PHE:HZ	1.79	0.46
1:B:239:LEU:HD12	1:B:239:LEU:HA	1.51	0.46
1:C:67:GLU:CD	1:F:104:THR:HG23	2.41	0.46
1:F:190:THR:C	1:F:192:MET:H	2.24	0.46
1:A:172:GLU:HG2	1:B:150:MET:HG3	1.97	0.46
1:C:133:ARG:HG2	1:C:176:ARG:HB3	1.97	0.46
1:E:2:GLN:OE1	1:E:229:ASP:HB2	2.16	0.46
1:E:154:ASN:OD1	1:E:155:TYR:N	2.47	0.46
1:C:97:LYS:HB2	1:C:102:MET:HE3	1.97	0.46
1:D:86:TYR:HB3	1:D:227:LEU:HD22	1.97	0.46
1:E:122:CYS:C	1:E:169:PHE:HE2	2.23	0.46
1:A:94:VAL:O	1:A:94:VAL:HG23	2.15	0.45
1:A:150:MET:HG3	1:B:172:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:HG22	1:B:124:GLU:OE2	2.16	0.45
1:C:188:ILE:C	1:C:190:THR:H	2.23	0.45
1:D:20:GLU:OE1	1:D:23:ARG:HD2	2.16	0.45
1:D:179:ARG:NH1	1:D:231:SER:O	2.49	0.45
1:C:221:GLU:OE1	1:D:230:HIS:HD2	1.99	0.45
1:F:24:THR:O	1:F:28:MET:HG3	2.16	0.45
1:A:24:THR:HG23	1:A:28:MET:HE3	1.98	0.45
1:A:27:SER:HA	1:A:55:TYR:CZ	2.51	0.45
1:A:140:ILE:O	1:A:159:LYS:NZ	2.46	0.45
1:C:221:GLU:OE1	1:D:230:HIS:CD2	2.69	0.45
1:F:144:ILE:HD12	1:F:152:GLN:NE2	2.31	0.45
2:G:59:ALA:HA	2:G:62:ILE:HD12	1.98	0.45
1:C:47:LYS:HE2	1:C:51:GLU:OE1	2.17	0.45
1:F:20:GLU:HG3	1:F:216:ALA:HB3	1.98	0.45
1:E:182:SER:HB2	1:E:238:THR:HG23	1.99	0.45
1:C:70:PHE:HE1	1:C:74:ILE:HD11	1.81	0.45
1:E:17:ILE:HB	3:E:301:NAP:O5D	2.17	0.45
1:A:24:THR:O	1:A:28:MET:HG3	2.17	0.45
1:B:219:VAL:O	1:B:223:VAL:HG23	2.16	0.45
1:C:215:ALA:HB3	1:C:218:GLU:HG3	1.99	0.45
1:F:116:THR:O	1:F:120:ILE:HG13	2.16	0.45
2:G:56:ASP:O	2:G:57:GLU:C	2.60	0.45
1:B:7:ASN:OD1	1:B:7:ASN:N	2.50	0.45
1:D:107:PHE:CE1	1:D:154:ASN:HA	2.52	0.45
1:F:87:LEU:HD23	1:F:88:VAL:N	2.32	0.45
1:F:146:GLU:OE2	1:F:184:THR:HG21	2.16	0.45
2:G:5:GLU:O	2:G:8:GLN:HB2	2.16	0.45
1:F:11:THR:O	1:F:90:ASN:HB3	2.17	0.44
1:B:6:LYS:HE2	1:B:6:LYS:HA	2.00	0.44
1:C:70:PHE:CD1	1:C:70:PHE:C	2.94	0.44
1:D:131:LYS:C	1:D:133:ARG:HH11	2.23	0.44
1:E:62:PHE:CD2	1:E:70:PHE:HA	2.52	0.44
1:E:74:ILE:C	1:E:77:ILE:HG22	2.40	0.44
1:E:42:VAL:O	1:E:45:ALA:HB3	2.17	0.44
1:F:137:VAL:HB	1:F:180:PHE:HD1	1.81	0.44
1:A:167:LYS:O	1:A:171:TYR:CD1	2.71	0.44
1:F:92:GLY:HA2	1:F:114:ASN:OD1	2.17	0.44
1:A:208:ILE:HG22	1:A:211:ASN:H	1.82	0.44
1:E:67:GLU:O	1:E:71:VAL:HG23	2.17	0.44
1:A:142:SER:HB3	1:A:159:LYS:HG3	1.99	0.44
1:E:2:GLN:O	1:E:228:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ASP:HA	1:F:116:THR:OG1	2.17	0.44
2:G:55:PRO:O	2:G:56:ASP:C	2.60	0.44
1:A:17:ILE:HD11	1:A:188:ILE:HG21	2.00	0.44
1:D:20:GLU:OE1	1:D:20:GLU:HA	2.18	0.44
1:F:125:ALA:O	1:F:129:MET:HB2	2.18	0.44
1:C:47:LYS:HD3	1:C:47:LYS:C	2.42	0.44
1:D:17:ILE:CD1	1:D:188:ILE:HG13	2.43	0.44
1:D:138:VAL:HG21	1:D:223:VAL:HG12	1.98	0.44
1:A:219:VAL:O	1:A:223:VAL:HG23	2.18	0.43
1:B:103:LYS:HB2	1:B:103:LYS:HE3	1.71	0.43
1:D:31:LYS:HD3	1:D:33:TRP:HE1	1.82	0.43
1:F:17:ILE:HD13	3:F:301:NAP:C5D	2.48	0.43
1:A:23:ARG:NH1	1:A:49:GLU:OE1	2.50	0.43
1:A:67:GLU:O	1:A:71:VAL:HG23	2.18	0.43
1:B:62:PHE:CE2	1:B:70:PHE:CG	3.03	0.43
1:F:35:ASN:ND2	3:F:301:NAP:H2A	2.33	0.43
1:F:247:MET:HE3	1:F:247:MET:HB3	1.57	0.43
1:A:212:ARG:HH22	1:A:218:GLU:CD	2.26	0.43
1:D:77:ILE:CG2	1:D:84:LEU:HB2	2.42	0.43
1:E:226:LEU:HD11	1:E:239:LEU:CD1	2.47	0.43
1:A:123:ARG:HE	1:A:123:ARG:HB3	1.54	0.43
1:C:24:THR:HG22	1:C:28:MET:HE3	2.01	0.43
1:C:110:VAL:HG11	1:C:154:ASN:HD22	1.83	0.43
1:C:154:ASN:CG	1:C:155:TYR:N	2.77	0.43
1:E:8:VAL:HG23	1:E:86:TYR:HB2	2.00	0.43
1:E:171:TYR:HD1	1:E:171:TYR:H	1.66	0.43
1:F:31:LYS:HD3	1:F:33:TRP:HE1	1.83	0.43
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.74	0.43
1:E:132:SER:O	1:E:133:ARG:HB2	2.18	0.43
2:G:43:ILE:HD12	2:G:62:ILE:HD13	1.99	0.43
1:A:41:GLU:H	1:A:41:GLU:HG3	1.56	0.43
1:C:1:MET:CE	1:C:225:PHE:HA	2.35	0.43
1:D:150:MET:CG	1:E:172:GLU:HG2	2.48	0.43
1:C:119:PHE:HB2	1:C:165:MET:SD	2.59	0.43
1:F:180:PHE:H	1:F:235:THR:HG23	1.83	0.43
2:G:51:GLY:HA3	2:G:72:ILE:HD11	2.01	0.43
1:B:87:LEU:HD23	1:B:88:VAL:N	2.33	0.43
2:G:19:ALA:O	2:G:22:VAL:HG22	2.18	0.43
1:A:21:ILE:HA	1:A:220:ALA:HB1	2.01	0.42
1:F:23:ARG:HG3	1:F:50:LEU:HD21	2.01	0.42
2:G:36:SER:O	2:G:38:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HE2	3:A:301:NAP:C3B	2.47	0.42
1:F:36:TYR:CD1	1:F:60:ILE:O	2.72	0.42
2:G:49:LYS:HD2	2:G:49:LYS:O	2.20	0.42
1:A:87:LEU:HD23	1:A:88:VAL:N	2.34	0.42
1:C:70:PHE:O	1:C:70:PHE:CD1	2.70	0.42
1:D:8:VAL:HG11	1:D:25:LEU:HD12	2.01	0.42
1:D:212:ARG:O	1:D:213:LEU:HD23	2.20	0.42
1:F:30:LEU:HD12	1:F:30:LEU:HA	1.82	0.42
1:C:139:ASN:HB3	1:C:162:MET:HE2	1.94	0.42
1:D:215:ALA:HB3	1:D:218:GLU:HG3	2.01	0.42
1:E:138:VAL:HG21	1:E:223:VAL:CG1	2.48	0.42
1:F:107:PHE:CE1	1:F:111:ILE:HG13	2.55	0.42
2:G:24:PRO:HA	2:G:65:VAL:HG23	2.01	0.42
1:C:41:GLU:OE1	1:C:41:GLU:CA	2.68	0.42
1:D:36:TYR:CD2	1:D:40:ALA:HA	2.54	0.42
1:F:26:ALA:HB1	1:F:55:TYR:HB3	2.01	0.42
1:B:11:THR:HA	1:B:35:ASN:HD22	1.84	0.42
1:B:11:THR:O	1:B:90:ASN:HB3	2.20	0.42
1:F:33:TRP:HA	1:F:58:ALA:O	2.18	0.42
2:G:46:LEU:N	2:G:46:LEU:HD12	2.34	0.42
1:C:240:LYS:HE3	1:D:237:GLU:OE2	2.20	0.42
1:D:165:MET:HB2	1:E:157:ALA:HB2	2.01	0.42
1:E:128:VAL:HG13	1:E:129:MET:HG3	2.01	0.42
1:F:131:LYS:N	1:F:131:LYS:HD2	2.34	0.42
3:C:301:NAP:H52A	3:C:301:NAP:H52N	2.01	0.42
1:D:203:ASP:HA	1:D:206:LYS:HZ2	1.85	0.42
1:B:8:VAL:HG23	1:B:86:TYR:HB2	2.01	0.42
1:B:112:ASP:HA	1:B:116:THR:OG1	2.20	0.42
1:C:1:MET:HB3	1:C:1:MET:HE2	1.83	0.42
1:C:95:ARG:NH1	1:C:106:ASP:OD1	2.50	0.42
1:D:104:THR:HG23	1:E:67:GLU:OE1	2.20	0.42
1:E:150:MET:HE2	1:E:150:MET:HB3	1.87	0.42
1:F:226:LEU:HD23	1:F:226:LEU:HA	1.84	0.42
1:D:130:SER:O	1:D:133:ARG:HD2	2.20	0.42
1:C:1:MET:HB2	1:C:28:MET:SD	2.60	0.41
1:D:22:ALA:O	1:D:23:ARG:C	2.62	0.41
1:E:93:VAL:HG11	1:E:113:ASN:HD22	1.85	0.41
1:E:130:SER:O	1:E:176:ARG:NH1	2.53	0.41
1:F:128:VAL:HG13	1:F:129:MET:HG3	2.02	0.41
2:G:23:THR:O	2:G:26:ALA:N	2.53	0.41
1:B:31:LYS:HE2	1:B:81:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PHE:HD1	1:C:70:PHE:C	2.28	0.41
1:E:39:ASN:HD21	1:E:42:VAL:CG2	2.32	0.41
1:E:169:PHE:CD2	1:E:180:PHE:CE2	3.06	0.41
2:G:49:LYS:O	2:G:49:LYS:CG	2.68	0.41
1:B:36:TYR:CE2	1:B:40:ALA:HB2	2.56	0.41
1:E:39:ASN:OD1	1:E:40:ALA:N	2.53	0.41
1:B:142:SER:C	1:B:184:THR:HB	2.45	0.41
1:D:141:ALA:CA	1:D:162:MET:HE1	2.51	0.41
1:F:124:GLU:O	1:F:128:VAL:HG12	2.20	0.41
2:G:42:LEU:O	2:G:46:LEU:HD13	2.20	0.41
2:G:52:ILE:HD12	2:G:53:GLU:CB	2.50	0.41
1:E:141:ALA:HA	1:E:162:MET:CE	2.50	0.41
2:G:22:VAL:HG23	2:G:22:VAL:O	2.20	0.41
1:B:27:SER:HA	1:B:55:TYR:CE1	2.55	0.41
1:C:135:GLY:O	1:C:178:ILE:HA	2.20	0.41
1:C:144:ILE:HD13	1:C:149:ASN:HB2	2.01	0.41
2:G:50:PHE:CD1	2:G:52:ILE:HG22	2.56	0.41
2:G:58:GLN:HB3	2:G:71:TYR:CD1	2.55	0.41
1:C:90:ASN:O	1:C:91:ALA:C	2.64	0.41
1:D:10:ILE:HG23	1:D:88:VAL:HB	2.03	0.41
1:D:46:LEU:C	1:D:46:LEU:CD2	2.93	0.41
1:D:150:MET:HB3	1:D:150:MET:HE2	1.71	0.41
1:E:88:VAL:HG13	1:E:138:VAL:CG2	2.51	0.41
2:G:42:LEU:O	2:G:45:ALA:HB3	2.21	0.41
1:C:247:MET:SD	1:D:171:TYR:CE1	3.14	0.40
1:D:7:ASN:OD1	1:D:7:ASN:N	2.54	0.40
1:D:56:LYS:HE2	1:D:56:LYS:HB2	1.84	0.40
2:G:28:PHE:O	2:G:33:GLY:N	2.54	0.40
2:G:36:SER:C	2:G:38:ASP:N	2.76	0.40
2:G:49:LYS:O	2:G:49:LYS:CD	2.70	0.40
1:C:116:THR:HG21	1:F:108:HIS:HE1	1.86	0.40
1:D:157:ALA:HB2	1:E:165:MET:HB2	2.02	0.40
1:F:84:LEU:HD21	1:F:86:TYR:O	2.22	0.40
1:C:17:ILE:HD11	1:C:188:ILE:HG13	2.02	0.40
1:E:241:VAL:HG13	1:F:234:ILE:HG12	2.03	0.40
1:A:118:ALA:C	1:A:165:MET:HE1	2.47	0.40
1:B:87:LEU:HB3	1:B:137:VAL:HG13	2.02	0.40
1:D:143:ILE:H	1:D:143:ILE:HG22	1.57	0.40
1:D:208:ILE:CD1	1:D:211:ASN:H	2.15	0.40
1:E:74:ILE:HA	1:E:77:ILE:CG2	2.48	0.40
1:A:74:ILE:O	1:A:78:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301:NAP:H52A	3:A:301:NAP:H52N	2.03	0.40
1:B:37:ARG:NH1	1:B:37:ARG:CB	2.72	0.40
1:C:39:ASN:OD1	1:C:39:ASN:N	2.52	0.40
1:C:191:ASP:OD1	1:C:192:MET:N	2.55	0.40
1:E:3:PHE:CE2	1:E:28:MET:HB3	2.56	0.40
1:E:141:ALA:N	1:E:183:VAL:O	2.38	0.40
1:F:47:LYS:HG2	1:F:57:ALA:CB	2.51	0.40
1:F:105:GLU:H	1:F:105:GLU:HG3	1.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
1	B	232/248 (94%)	219 (94%)	13 (6%)	0	100	100
1	C	235/248 (95%)	218 (93%)	17 (7%)	0	100	100
1	D	232/248 (94%)	210 (90%)	19 (8%)	3 (1%)	9	20
1	E	237/248 (96%)	221 (93%)	16 (7%)	0	100	100
1	F	235/248 (95%)	219 (93%)	15 (6%)	1 (0%)	30	48
2	G	71/78 (91%)	58 (82%)	12 (17%)	1 (1%)	9	18
All	All	1488/1566 (95%)	1382 (93%)	101 (7%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	100	ILE
1	D	77	ILE
1	D	99	ALA

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Mol	Chain	Res	Type
1	F	68	SER
2	G	35	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/197 (100%)	189 (96%)	8 (4%)	27	52
1	B	186/197 (94%)	177 (95%)	9 (5%)	23	46
1	C	189/197 (96%)	181 (96%)	8 (4%)	26	51
1	D	186/197 (94%)	177 (95%)	9 (5%)	23	46
1	E	191/197 (97%)	187 (98%)	4 (2%)	47	70
1	F	189/197 (96%)	182 (96%)	7 (4%)	30	55
2	G	62/65 (95%)	50 (81%)	12 (19%)	1	2
All	All	1200/1247 (96%)	1143 (95%)	57 (5%)	23	46

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	39	ASN
1	A	42	VAL
1	A	47	LYS
1	A	93	VAL
1	A	123	ARG
1	A	150	MET
1	A	240	LYS
1	B	4	THR
1	B	37	ARG
1	B	38	SER
1	B	39	ASN
1	B	41	GLU
1	B	42	VAL
1	B	229	ASP

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Mol	Chain	Res	Type
1	B	231	SER
1	B	232	SER
1	C	35	ASN
1	C	38	SER
1	C	41	GLU
1	C	42	VAL
1	C	71	VAL
1	C	140	ILE
1	C	143	ILE
1	C	144	ILE
1	D	39	ASN
1	D	42	VAL
1	D	116	THR
1	D	127	LYS
1	D	143	ILE
1	D	146	GLU
1	D	150	MET
1	D	208	ILE
1	D	237	GLU
1	E	39	ASN
1	E	97	LYS
1	E	162	MET
1	E	168	SER
1	F	37	ARG
1	F	56	LYS
1	F	94	VAL
1	F	140	ILE
1	F	142	SER
1	F	143	ILE
1	F	247	MET
2	G	15	LEU
2	G	17	VAL
2	G	18	ASP
2	G	36	SER
2	G	37	LEU
2	G	49	LYS
2	G	50	PHE
2	G	52	ILE
2	G	54	ILE
2	G	58	GLN
2	G	60	GLU
2	G	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	89	ASN
1	A	113	ASN
1	A	139	ASN
1	A	193	ASN
1	B	35	ASN
1	B	89	ASN
1	B	113	ASN
1	B	230	HIS
1	C	35	ASN
1	C	152	GLN
1	C	154	ASN
1	D	35	ASN
1	D	89	ASN
1	D	207	ASN
1	D	230	HIS
1	E	48	ASN
1	E	75	GLN
1	E	114	ASN
1	E	139	ASN
1	F	89	ASN
1	F	152	GLN
1	F	230	HIS
2	G	14	GLN
2	G	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAP	A	301	-	50,52,52	1.22	5 (10%)	71,80,80	1.61	12 (16%)
3	NAP	E	301	-	50,52,52	0.62	1 (2%)	71,80,80	0.83	1 (1%)
3	NAP	B	301	-	50,52,52	1.41	7 (14%)	71,80,80	1.43	9 (12%)
3	NAP	D	301	-	50,52,52	0.65	1 (2%)	71,80,80	0.80	2 (2%)
4	UHC	G	101	-	24,30,31	0.68	0	30,38,41	2.27	8 (26%)
3	NAP	F	301	-	50,52,52	0.63	1 (2%)	71,80,80	0.78	1 (1%)
3	NAP	C	301	-	50,52,52	1.11	4 (8%)	71,80,80	1.73	15 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	301	-	-	12/35/67/67	0/5/5/5
3	NAP	E	301	-	-	8/35/67/67	0/5/5/5
3	NAP	B	301	-	-	7/35/67/67	0/5/5/5
3	NAP	D	301	-	-	11/35/67/67	0/5/5/5
4	UHC	G	101	-	-	18/36/38/39	-
3	NAP	F	301	-	-	12/35/67/67	0/5/5/5
3	NAP	C	301	-	-	5/35/67/67	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAP	P2B-O2B	-5.37	1.50	1.59
3	C	301	NAP	C6N-N1N	-4.17	1.25	1.35
3	A	301	NAP	PA-O3	3.76	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NAP	C6N-N1N	-3.70	1.26	1.35
3	B	301	NAP	PN-O3	-3.47	1.55	1.59
3	A	301	NAP	C2N-N1N	3.32	1.38	1.35
3	B	301	NAP	C4N-C3N	-3.07	1.34	1.39
3	C	301	NAP	PA-O3	2.88	1.62	1.59
3	E	301	NAP	C2N-N1N	2.74	1.38	1.35
3	B	301	NAP	C5N-C4N	-2.73	1.34	1.38
3	D	301	NAP	C2N-N1N	2.66	1.37	1.35
3	A	301	NAP	PN-O3	2.63	1.62	1.59
3	F	301	NAP	C2N-N1N	2.60	1.37	1.35
3	C	301	NAP	C4N-C3N	-2.38	1.35	1.39
3	B	301	NAP	P2B-O2X	-2.28	1.46	1.54
3	B	301	NAP	PA-O3	-2.23	1.57	1.59
3	A	301	NAP	C4N-C3N	-2.20	1.36	1.39
3	B	301	NAP	P2B-O3X	-2.19	1.46	1.54
3	C	301	NAP	O4D-C4D	-2.06	1.40	1.45

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	NAP	O2B-C2B-C3B	6.42	134.69	111.68
3	C	301	NAP	C6N-N1N-C2N	-5.85	116.90	121.88
4	G	101	UHC	C30-C29-C32	5.40	117.97	108.77
3	E	301	NAP	P2B-O2B-C2B	-5.28	109.32	123.43
4	G	101	UHC	O1-C1-S1	5.09	129.16	122.68
3	B	301	NAP	O2B-C2B-C1B	-4.98	92.53	110.05
4	G	101	UHC	C3-C2-C1	-4.93	102.97	112.45
3	C	301	NAP	C2B-C1B-N9A	4.92	121.85	113.75
3	F	301	NAP	P2B-O2B-C2B	-4.81	110.60	123.43
3	D	301	NAP	P2B-O2B-C2B	-4.65	111.00	123.43
3	B	301	NAP	P2B-O2B-C2B	-4.50	111.42	123.43
4	G	101	UHC	O1-C1-C2	-4.37	116.12	123.40
3	A	301	NAP	O2D-C2D-C3D	-4.27	98.13	111.82
3	C	301	NAP	O2B-C2B-C3B	3.96	125.89	111.68
3	B	301	NAP	C6N-N1N-C2N	-3.96	118.51	121.88
4	G	101	UHC	C5-C4-C3	-3.79	104.99	114.59
3	C	301	NAP	O2D-C2D-C3D	-3.76	99.77	111.82
3	C	301	NAP	C5N-C4N-C3N	-3.71	116.71	120.36
3	C	301	NAP	O2B-C2B-C1B	3.68	123.01	110.05
3	A	301	NAP	C5N-C4N-C3N	-3.61	116.82	120.36
3	B	301	NAP	O4B-C1B-N9A	3.51	114.84	108.09
3	C	301	NAP	P2B-O2B-C2B	3.40	132.51	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAP	O3B-C3B-C4B	-3.31	101.58	111.08
3	A	301	NAP	O2B-C2B-C1B	2.99	120.58	110.05
4	G	101	UHC	C42-N41-C39	2.87	128.16	122.82
3	A	301	NAP	O2X-P2B-O2B	-2.83	94.83	105.85
3	C	301	NAP	C3B-C2B-C1B	-2.76	97.51	102.81
3	A	301	NAP	C4D-O4D-C1D	-2.75	107.40	109.92
3	A	301	NAP	C6N-C5N-C4N	-2.75	115.49	119.45
3	B	301	NAP	C3B-C2B-C1B	-2.70	97.63	102.81
3	A	301	NAP	O4B-C1B-N9A	2.70	113.27	108.09
3	C	301	NAP	C4D-O4D-C1D	-2.62	107.52	109.92
4	G	101	UHC	C32-C34-N36	2.52	121.26	116.48
3	A	301	NAP	C6N-N1N-C2N	-2.49	119.76	121.88
3	B	301	NAP	O4B-C1B-C2B	-2.49	102.30	106.59
3	C	301	NAP	C5N-C6N-N1N	-2.45	117.04	120.38
3	C	301	NAP	O2X-P2B-O2B	-2.45	96.30	105.85
3	C	301	NAP	O3D-C3D-C4D	2.44	118.10	111.08
3	C	301	NAP	O2A-PA-O1A	2.37	123.45	112.44
3	D	301	NAP	C6N-N1N-C2N	-2.35	119.88	121.88
3	C	301	NAP	C6N-C5N-C4N	-2.34	116.08	119.45
3	A	301	NAP	O3D-C3D-C4D	2.33	117.79	111.08
3	A	301	NAP	P2B-O2B-C2B	2.29	129.56	123.43
4	G	101	UHC	C37-N36-C34	-2.27	118.47	122.55
3	C	301	NAP	O2N-PN-O3	2.23	113.31	107.27
3	A	301	NAP	O2A-PA-O1A	2.23	122.80	112.44
3	B	301	NAP	C4B-O4B-C1B	-2.09	104.86	109.47
3	B	301	NAP	C2N-N1N-C1D	2.01	123.57	119.13

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	NAP	C3B-C2B-O2B-P2B
3	A	301	NAP	O4D-C4D-C5D-O5D
3	A	301	NAP	C3D-C4D-C5D-O5D
3	B	301	NAP	C5D-O5D-PN-O3
3	B	301	NAP	C5D-O5D-PN-O1N
3	B	301	NAP	C5D-O5D-PN-O2N
3	B	301	NAP	O4D-C1D-N1N-C2N
3	D	301	NAP	C5B-O5B-PA-O1A
3	D	301	NAP	C5D-O5D-PN-O1N
3	D	301	NAP	C5D-O5D-PN-O2N
3	D	301	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	D	301	NAP	C2D-C1D-N1N-C6N
3	E	301	NAP	O4D-C4D-C5D-O5D
3	F	301	NAP	C5B-O5B-PA-O2A
3	F	301	NAP	C5D-O5D-PN-O1N
3	F	301	NAP	O4D-C1D-N1N-C2N
4	G	101	UHC	O1-C1-S1-C43
4	G	101	UHC	C2-C1-S1-C43
4	G	101	UHC	C28-C29-C32-O33
4	G	101	UHC	C30-C29-C32-O33
4	G	101	UHC	C38-C39-N41-C42
3	E	301	NAP	C3D-C4D-C5D-O5D
3	F	301	NAP	O4D-C4D-C5D-O5D
3	F	301	NAP	C3D-C4D-C5D-O5D
4	G	101	UHC	O3-C3-C4-C5
4	G	101	UHC	C2-C3-C4-C5
4	G	101	UHC	O40-C39-N41-C42
3	C	301	NAP	C1B-C2B-O2B-P2B
3	D	301	NAP	O4B-C4B-C5B-O5B
3	D	301	NAP	C3B-C4B-C5B-O5B
3	C	301	NAP	C3B-C2B-O2B-P2B
4	G	101	UHC	C5-C6-C7-C8
3	C	301	NAP	O4B-C4B-C5B-O5B
4	G	101	UHC	C31-C29-C32-O33
3	F	301	NAP	O4B-C4B-C5B-O5B
4	G	101	UHC	C1-C2-C3-O3
4	G	101	UHC	O33-C32-C34-O35
3	A	301	NAP	C2B-O2B-P2B-O1X
4	G	101	UHC	C42-C43-S1-C1
3	A	301	NAP	C5D-O5D-PN-O3
3	A	301	NAP	C5D-O5D-PN-O1N
3	A	301	NAP	C5D-O5D-PN-O2N
3	D	301	NAP	C5D-O5D-PN-O3
3	E	301	NAP	C5D-O5D-PN-O3
3	E	301	NAP	C5D-O5D-PN-O1N
3	E	301	NAP	C5D-O5D-PN-O2N
3	F	301	NAP	C5B-O5B-PA-O1A
3	F	301	NAP	C5B-O5B-PA-O3
4	G	101	UHC	N36-C37-C38-C39
3	A	301	NAP	PA-O3-PN-O2N
3	D	301	NAP	PN-O3-PA-O2A
3	E	301	NAP	C2B-O2B-P2B-O2X
3	A	301	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	B	301	NAP	C1B-C2B-O2B-P2B
3	C	301	NAP	O4D-C4D-C5D-O5D
4	G	101	UHC	C1-C2-C3-C4
4	G	101	UHC	O1-C1-C2-C3
3	A	301	NAP	O4D-C1D-N1N-C2N
3	B	301	NAP	O4D-C1D-N1N-C6N
3	C	301	NAP	O4D-C1D-N1N-C6N
3	F	301	NAP	C3B-C4B-C5B-O5B
3	F	301	NAP	O4D-C1D-N1N-C6N
3	B	301	NAP	C2B-O2B-P2B-O1X
3	A	301	NAP	PA-O3-PN-O1N
4	G	101	UHC	C31-C29-C32-C34
3	F	301	NAP	PA-O3-PN-O2N
3	E	301	NAP	O4B-C4B-C5B-O5B
3	A	301	NAP	C2B-O2B-P2B-O2X
3	D	301	NAP	C4B-C5B-O5B-PA
3	E	301	NAP	C2B-O2B-P2B-O1X
4	G	101	UHC	O33-C32-C34-N36
3	D	301	NAP	PA-O3-PN-O2N
3	F	301	NAP	PA-O3-PN-O1N

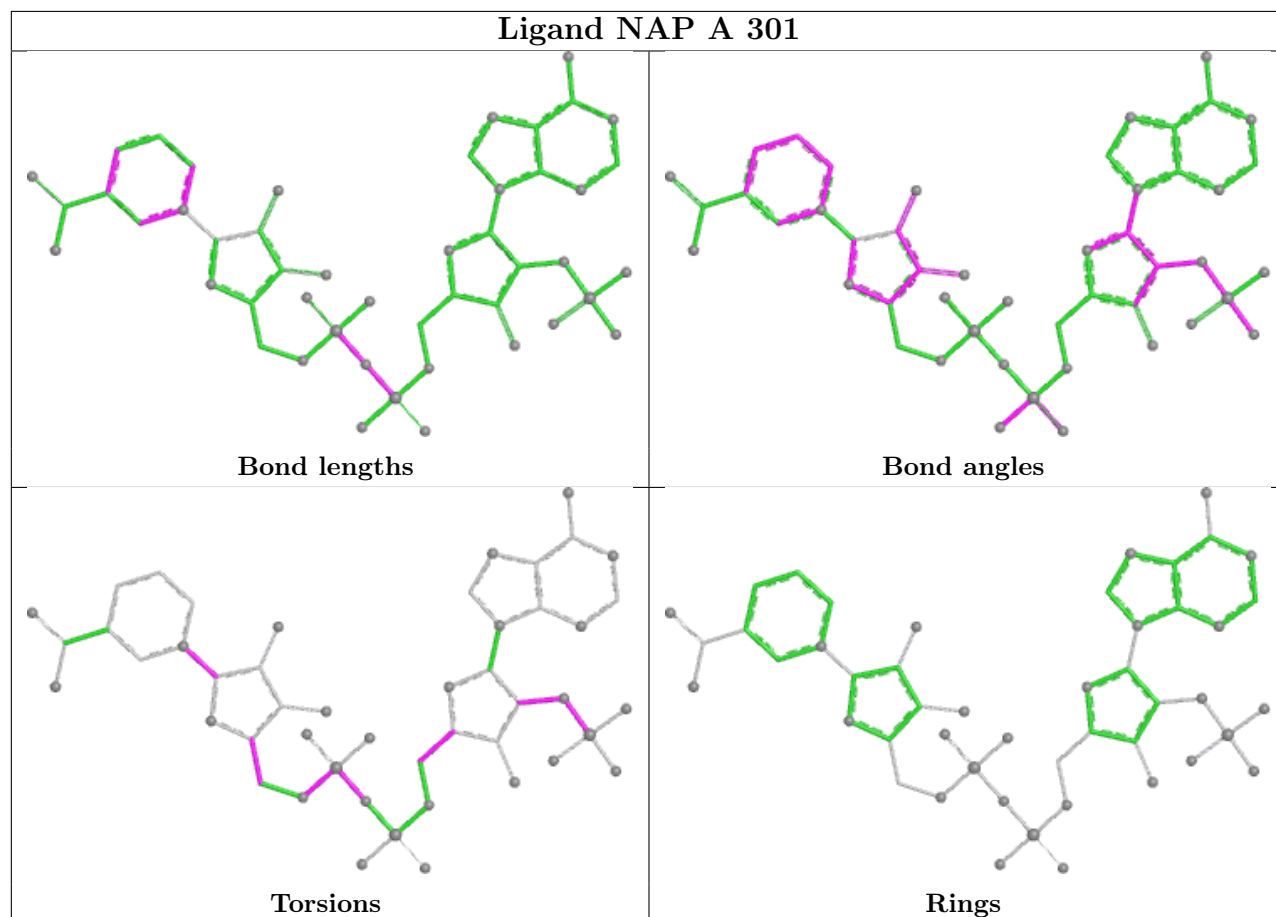
There are no ring outliers.

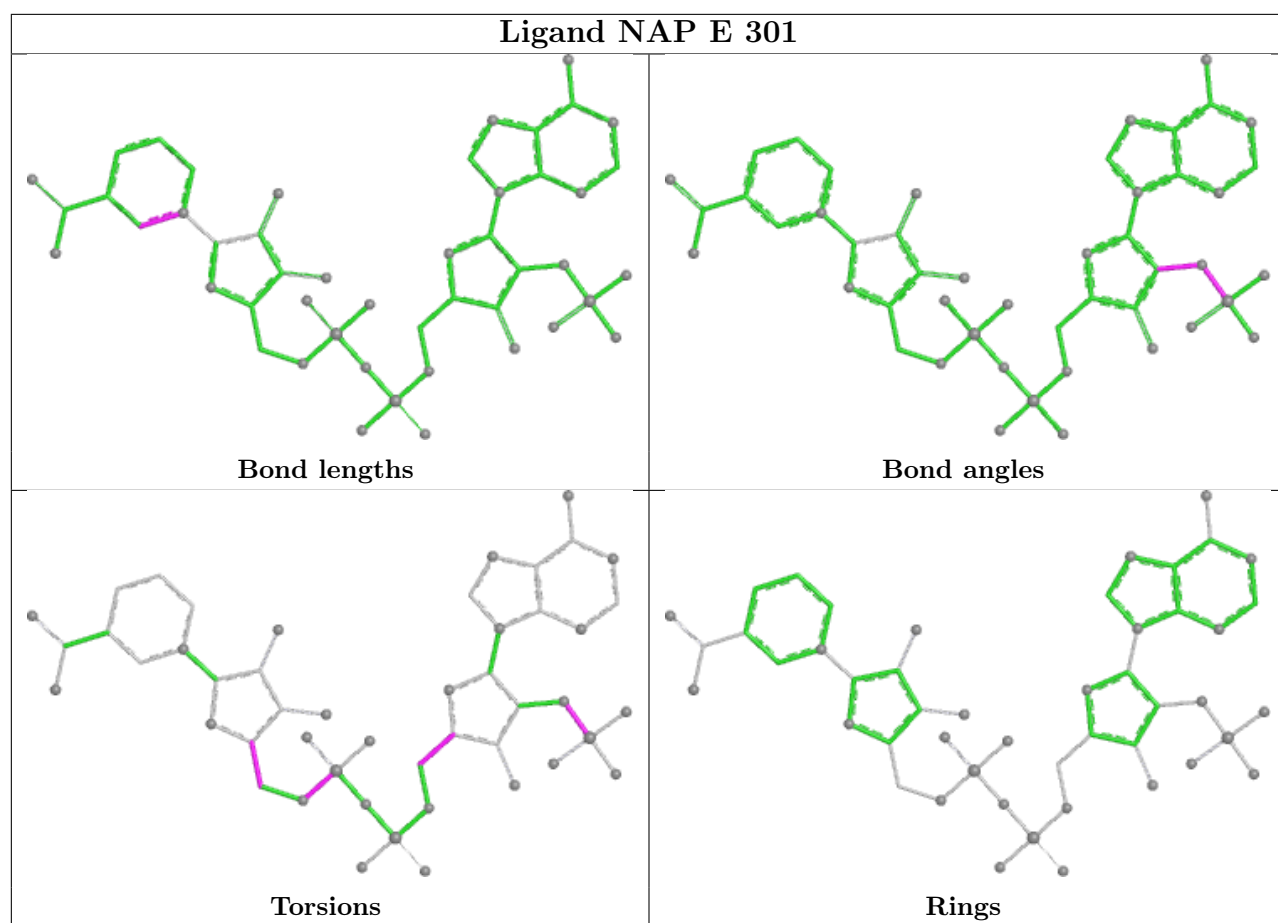
7 monomers are involved in 32 short contacts:

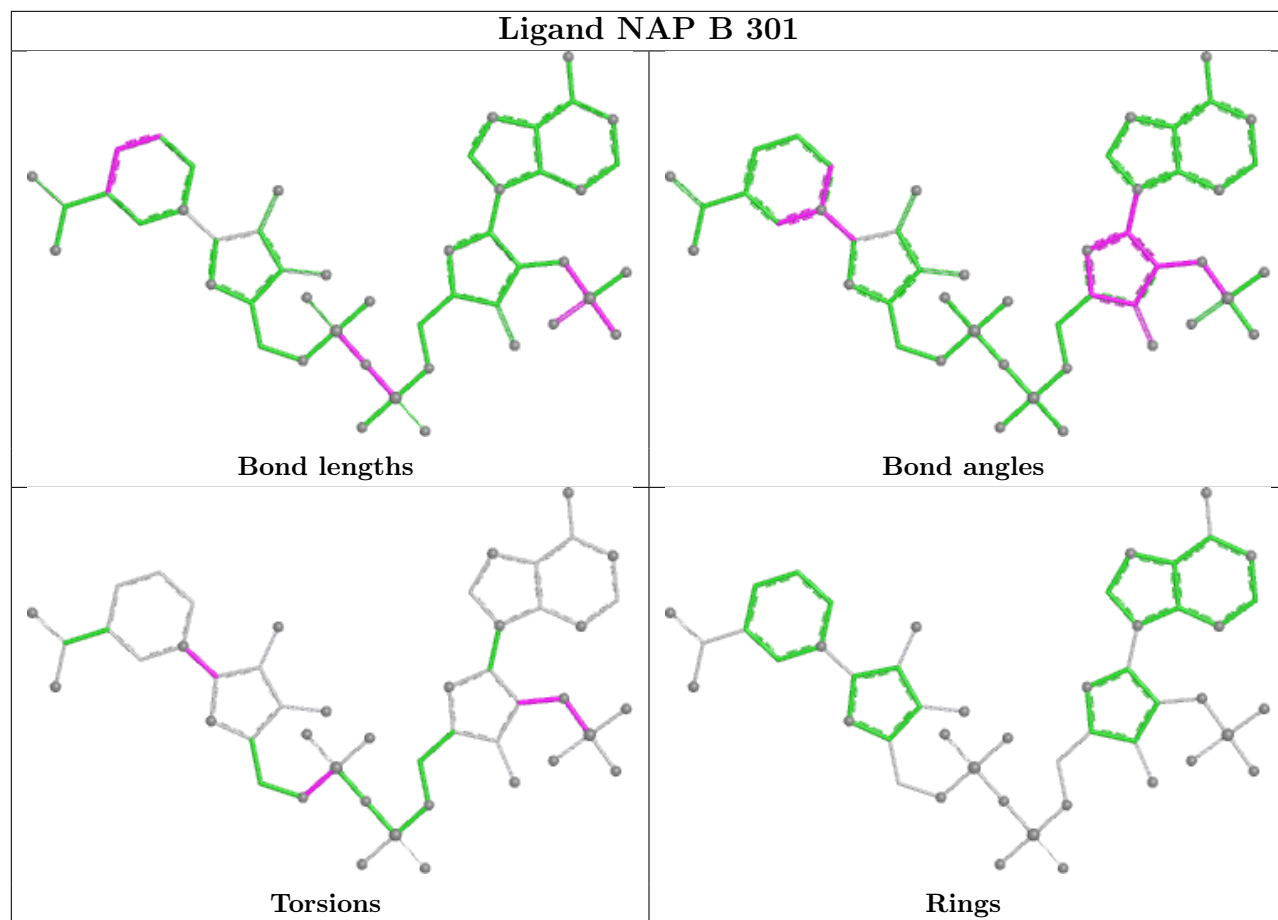
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAP	6	0
3	E	301	NAP	3	0
3	B	301	NAP	7	0
3	D	301	NAP	4	0
4	G	101	UHC	2	0
3	F	301	NAP	7	0
3	C	301	NAP	3	0

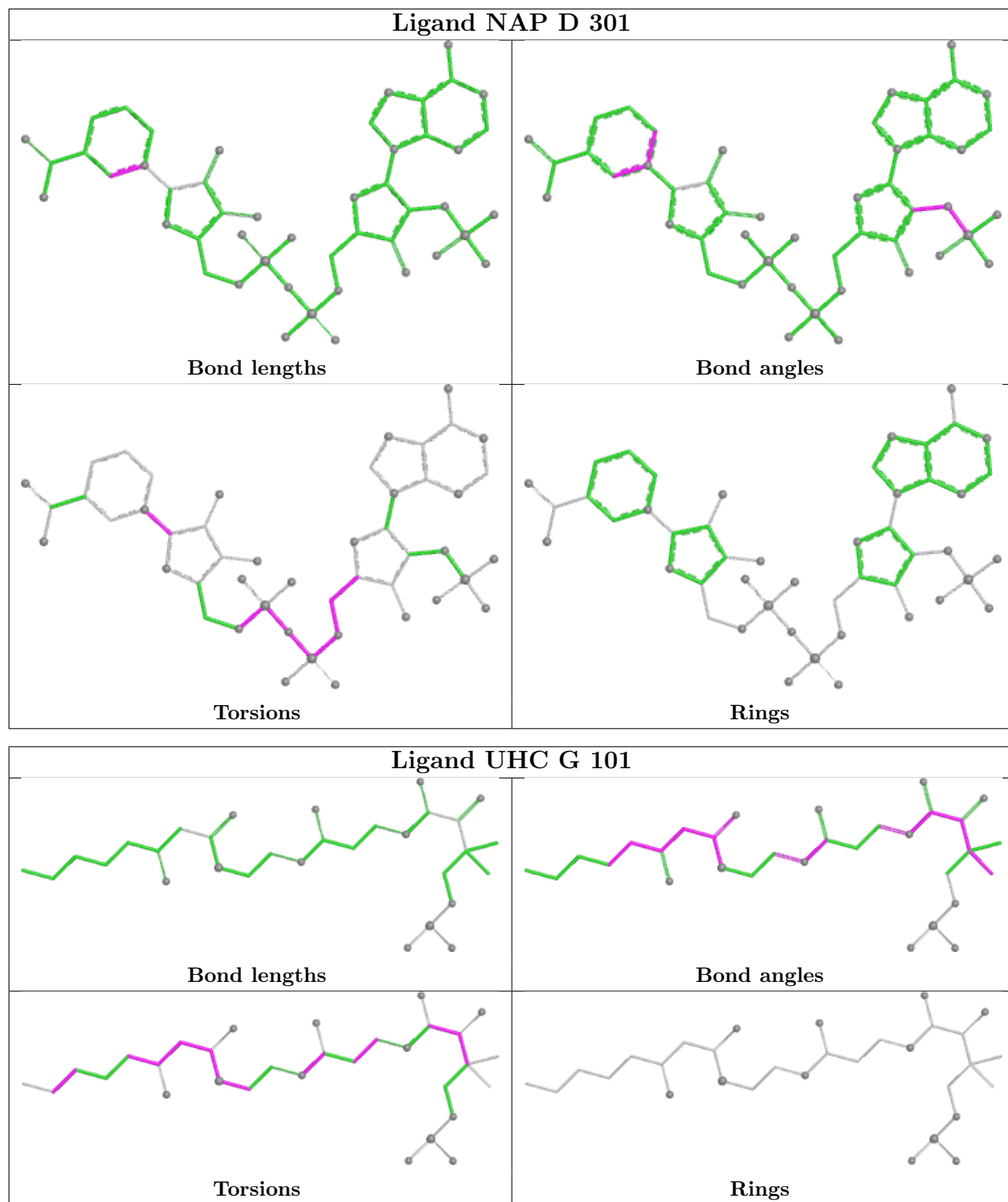
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

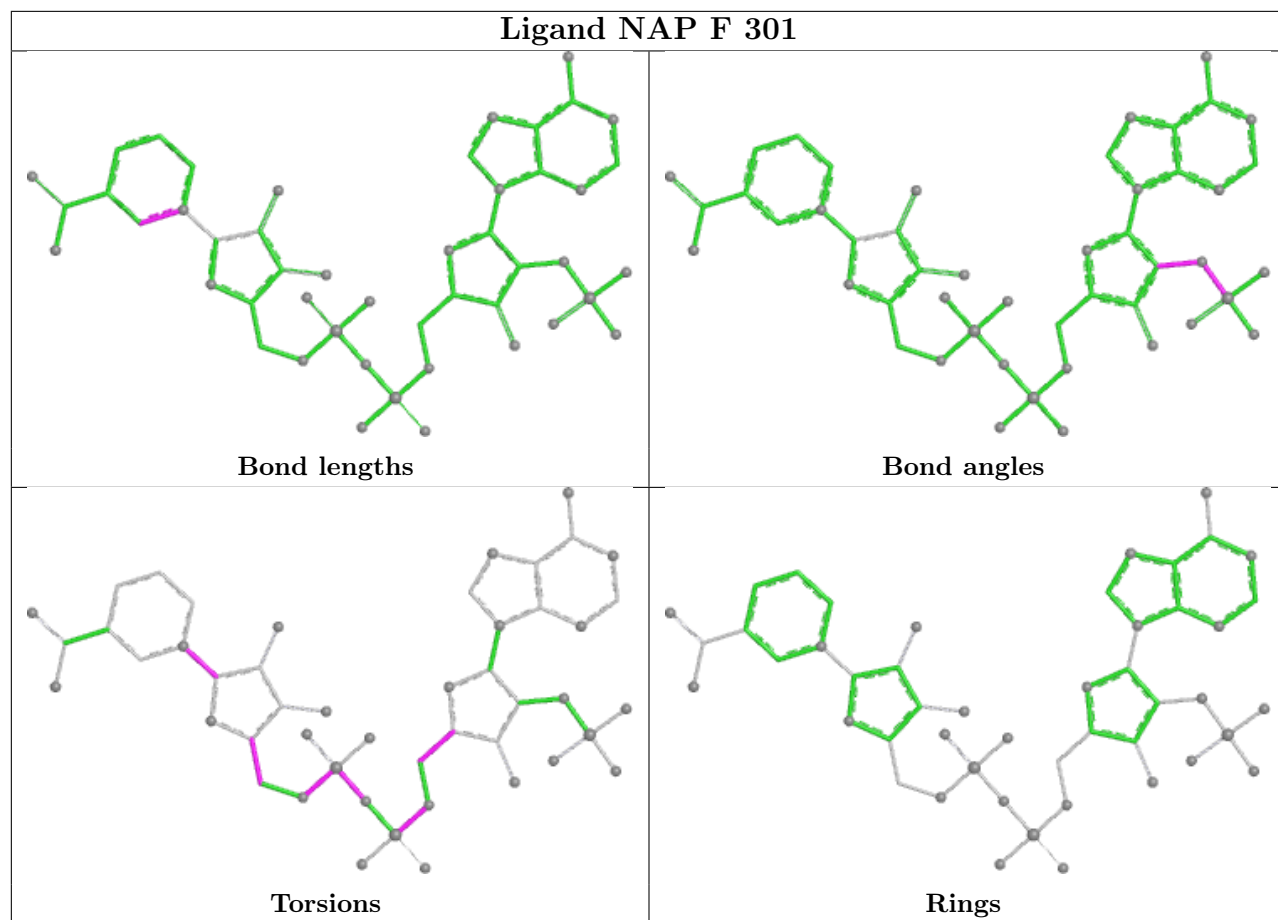
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

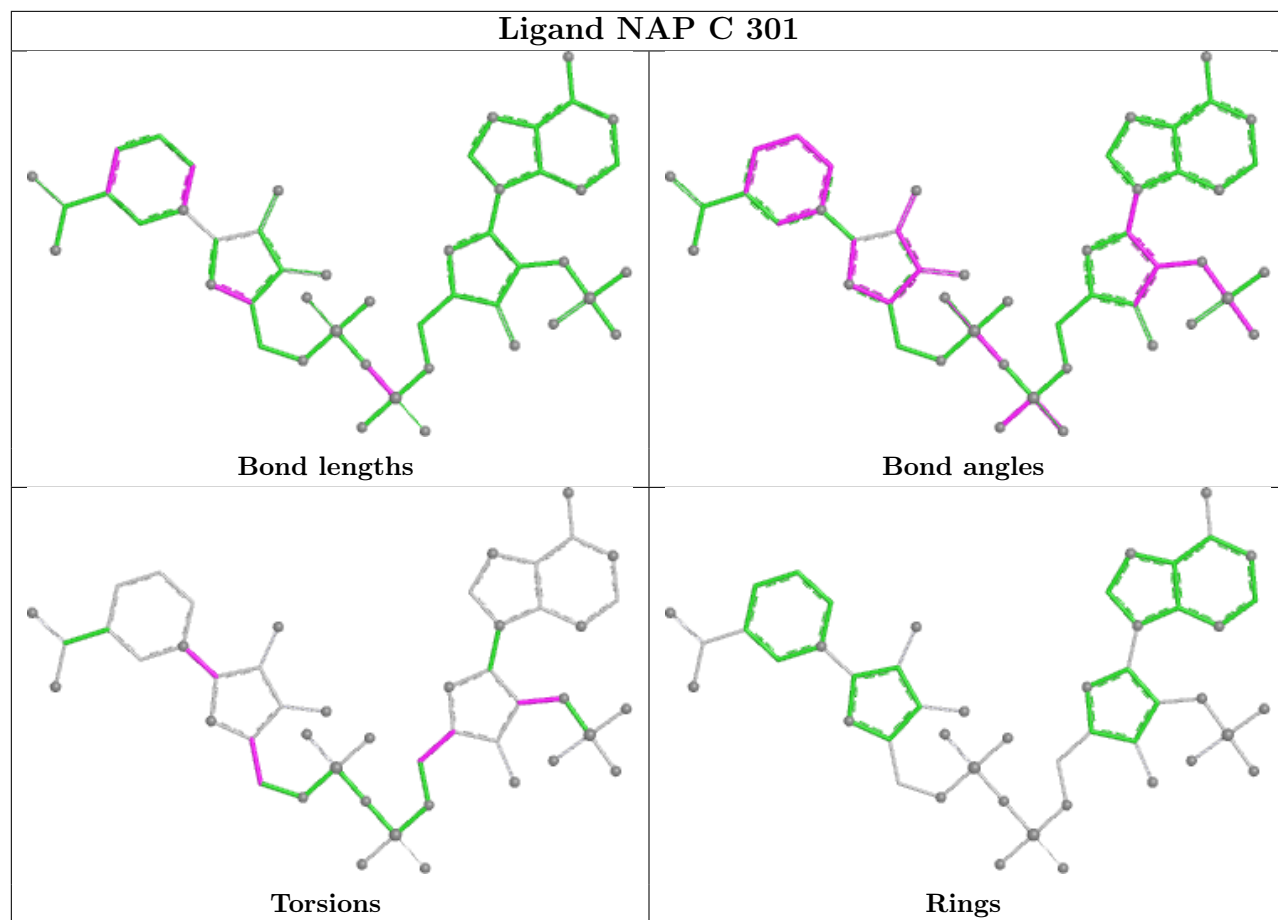












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/248 (100%)	0.29	5 (2%) 65 57	48, 64, 87, 116	0
1	B	236/248 (95%)	0.25	3 (1%) 75 69	50, 67, 88, 109	0
1	C	239/248 (96%)	0.50	5 (2%) 63 55	64, 83, 102, 121	0
1	D	236/248 (95%)	0.55	8 (3%) 48 38	62, 86, 112, 127	0
1	E	241/248 (97%)	0.50	7 (2%) 53 44	59, 80, 107, 131	0
1	F	239/248 (96%)	0.57	10 (4%) 40 32	66, 89, 107, 125	0
2	G	73/78 (93%)	0.42	1 (1%) 73 67	75, 114, 122, 128	0
All	All	1512/1566 (96%)	0.44	39 (2%) 57 48	48, 80, 111, 131	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	SER	4.3
1	D	202	ALA	3.8
1	A	68	SER	3.1
1	F	202	ALA	3.1
1	A	86	TYR	3.1
1	D	188	ILE	2.9
1	E	175	LEU	2.9
1	F	187	PHE	2.8
1	F	115	LEU	2.8
1	D	58	ALA	2.7
1	E	64	ALA	2.6
1	B	183	VAL	2.4
1	F	33	TRP	2.4
1	D	45	ALA	2.3
1	D	57	ALA	2.3
1	F	58	ALA	2.3
1	F	50	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	100	ILE	2.3
1	E	57	ALA	2.3
2	G	11	ILE	2.2
1	F	235	THR	2.2
1	D	204	TYR	2.2
1	A	57	ALA	2.2
1	D	73	ALA	2.2
1	C	115	LEU	2.1
1	C	112	ASP	2.1
1	D	84	LEU	2.1
1	E	105	GLU	2.1
1	E	158	SER	2.1
1	E	223	VAL	2.1
1	F	73	ALA	2.1
1	B	210	LEU	2.0
1	C	174	ALA	2.0
1	E	141	ALA	2.0
1	F	57	ALA	2.0
1	C	156	SER	2.0
1	A	236	GLY	2.0
1	A	58	ALA	2.0
1	B	57	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

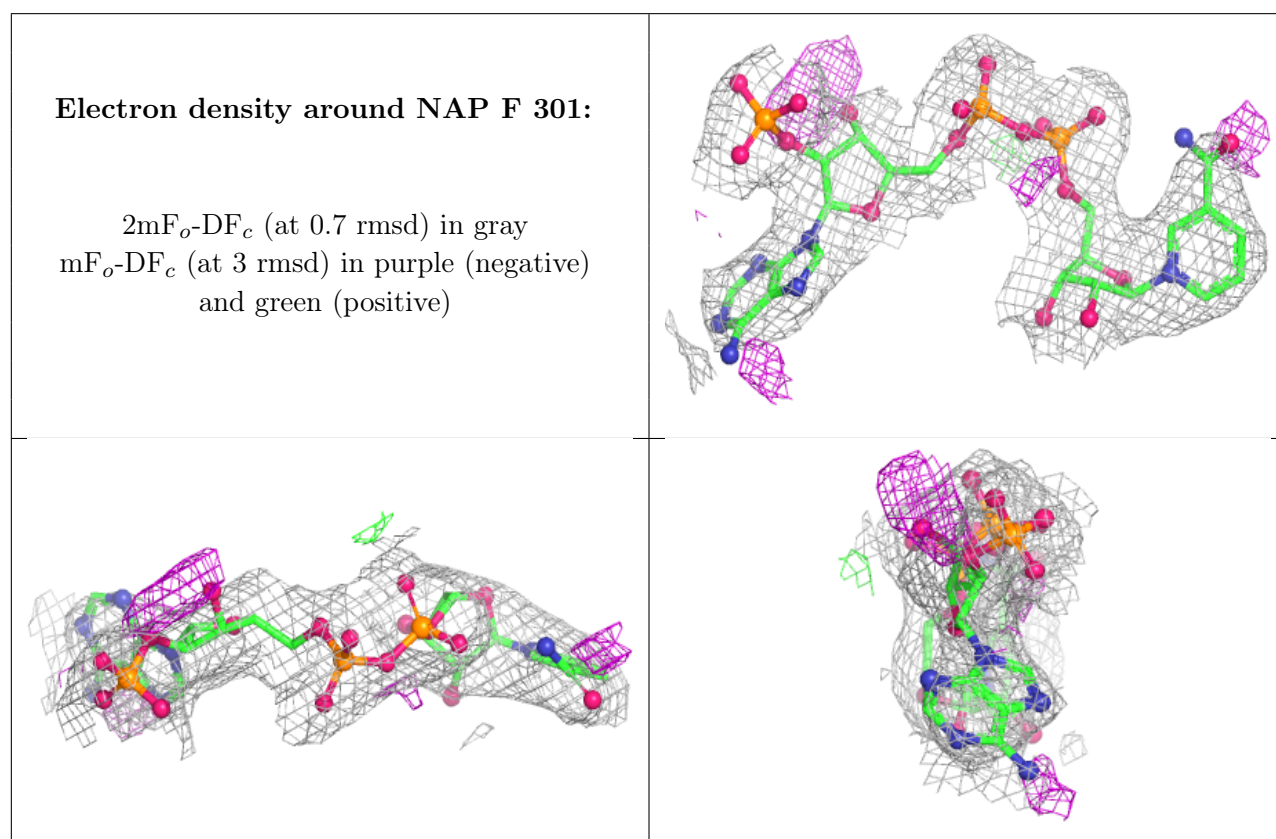
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	F	301	48/48	0.70	0.11	77,96,109,113	0

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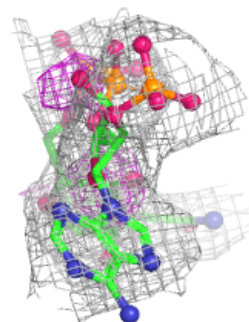
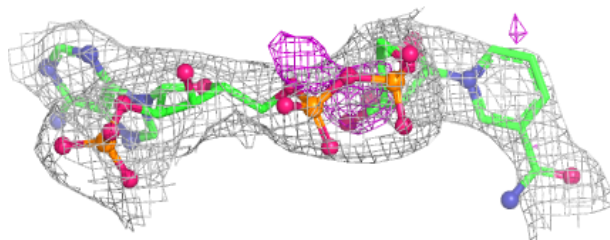
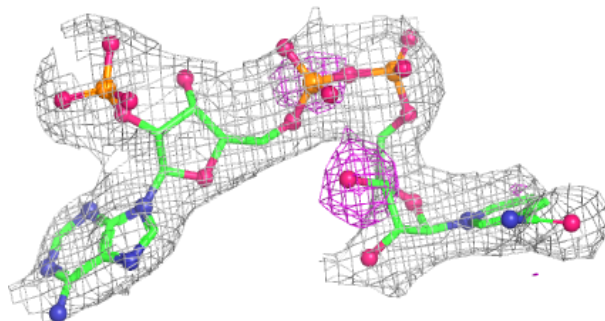
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	D	301	48/48	0.74	0.11	85,98,120,125	0
3	NAP	E	301	48/48	0.76	0.10	80,102,119,130	0
3	NAP	B	301	48/48	0.84	0.09	67,81,97,99	0
4	UHC	G	101	31/32	0.85	0.15	58,77,103,120	0
3	NAP	C	301	48/48	0.88	0.10	76,83,97,99	0
3	NAP	A	301	48/48	0.89	0.09	51,66,79,87	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

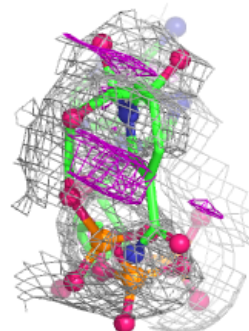
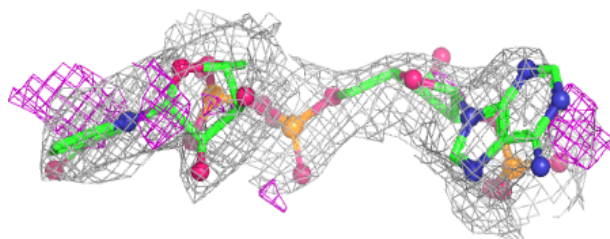
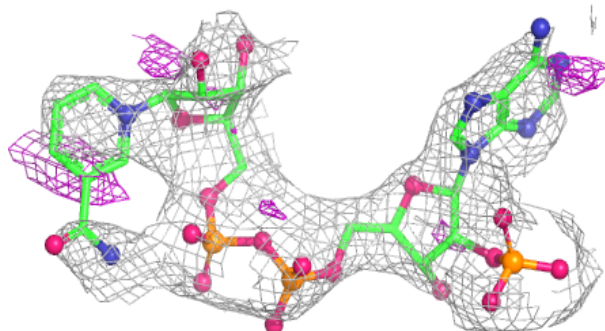


Electron density around NAP D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

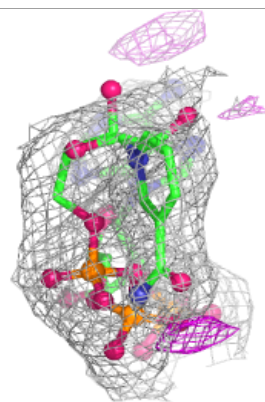
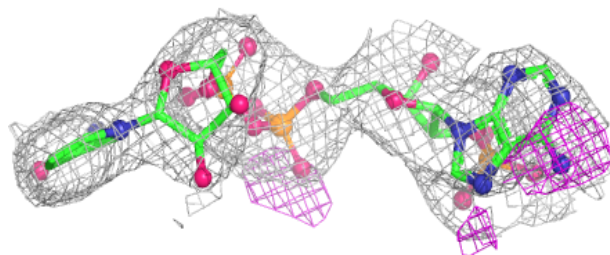
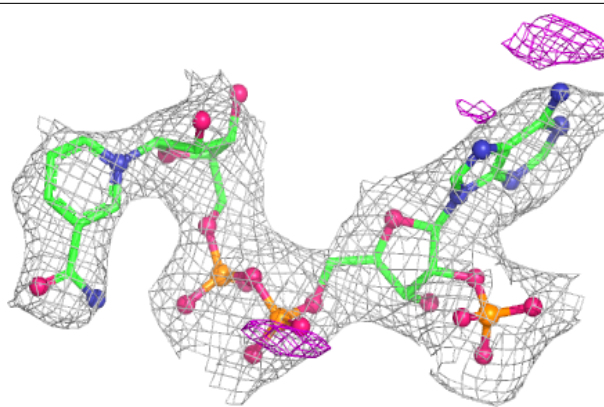
**Electron density around NAP E 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

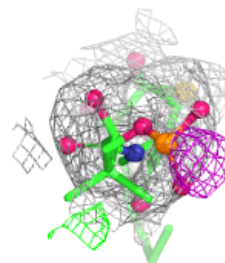
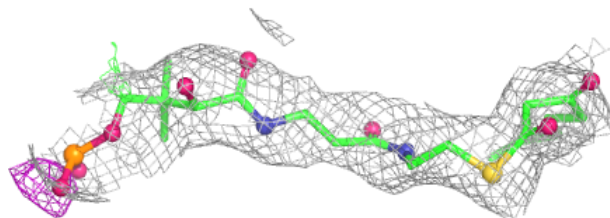
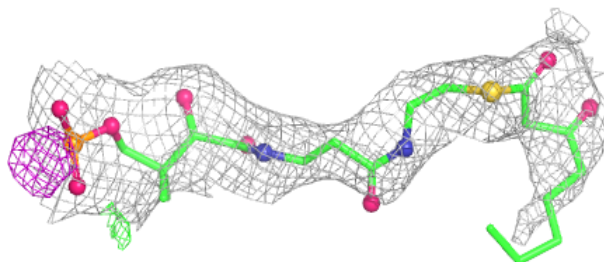


Electron density around NAP B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

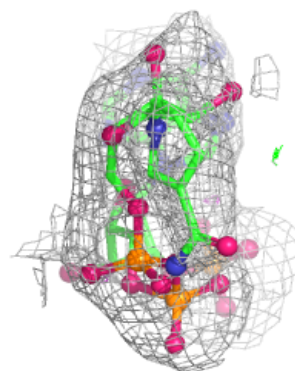
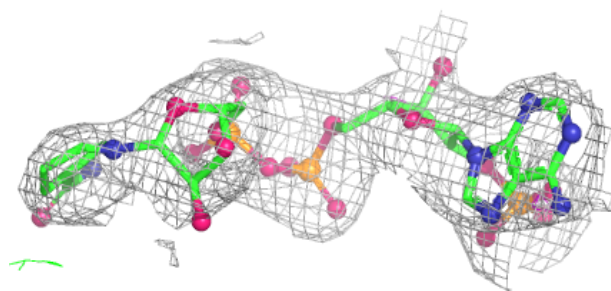
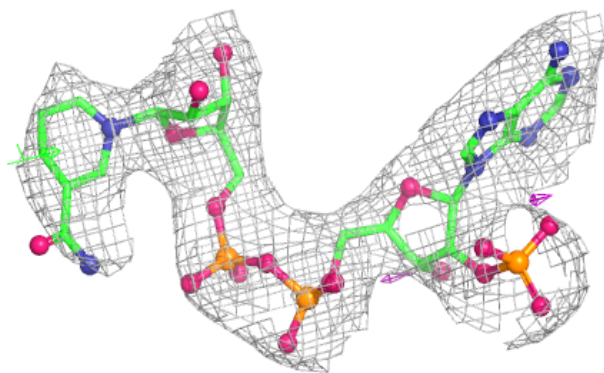
**Electron density around UHC G 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

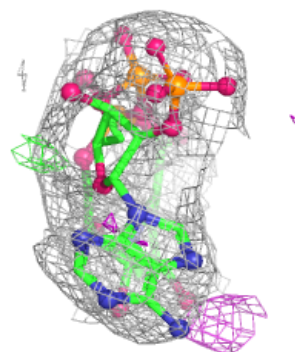
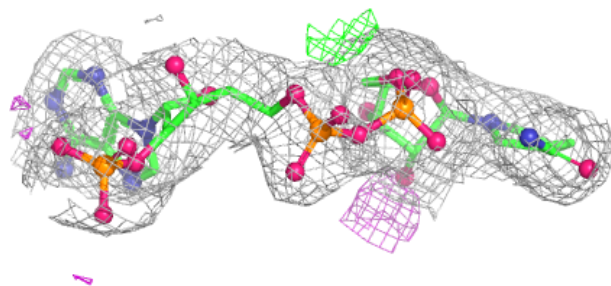
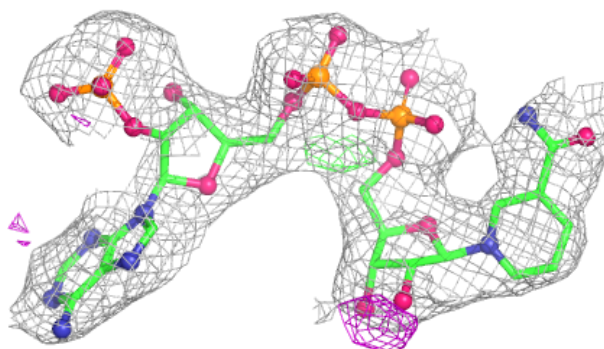


Electron density around NAP C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAP A 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.